

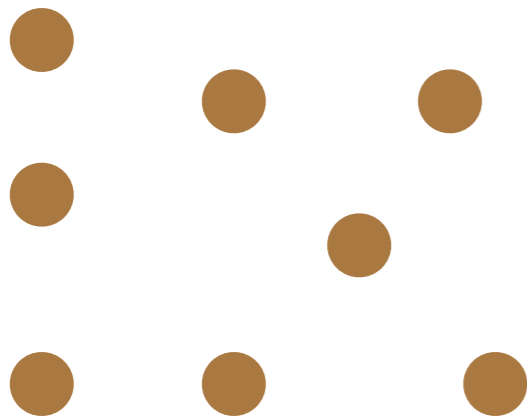
# Bayesian Data Analysis in Raman Spectroscopy

Vlad Vyshemirsky  
Department of Computing Science  
University of Glasgow

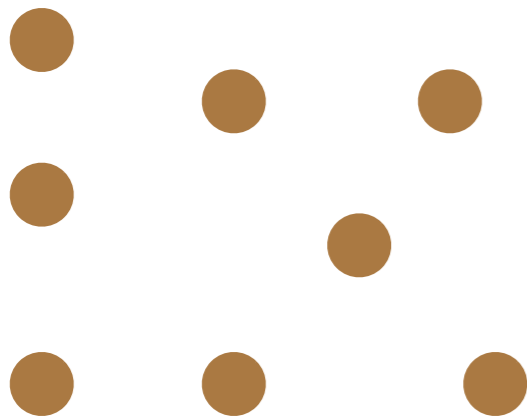


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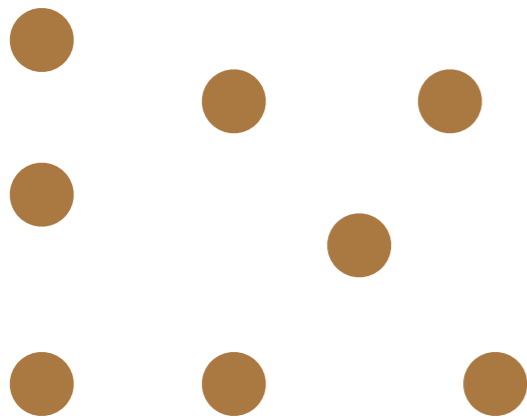
# Light Scattering



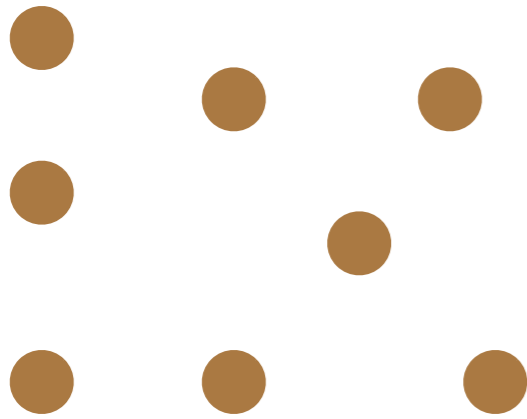
# Light Scattering



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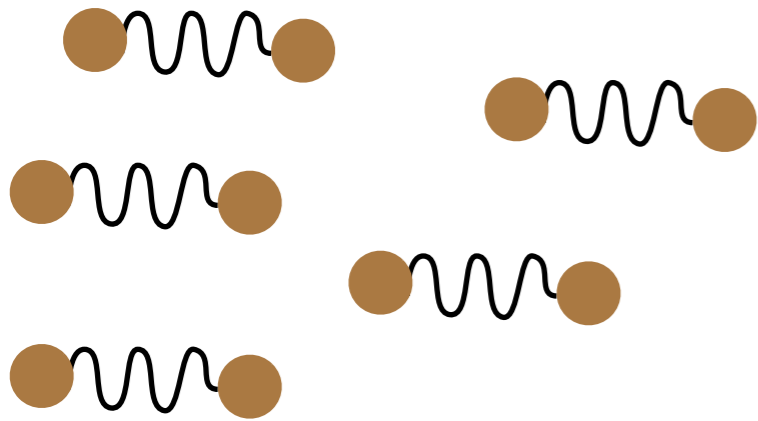


# Light Scattering

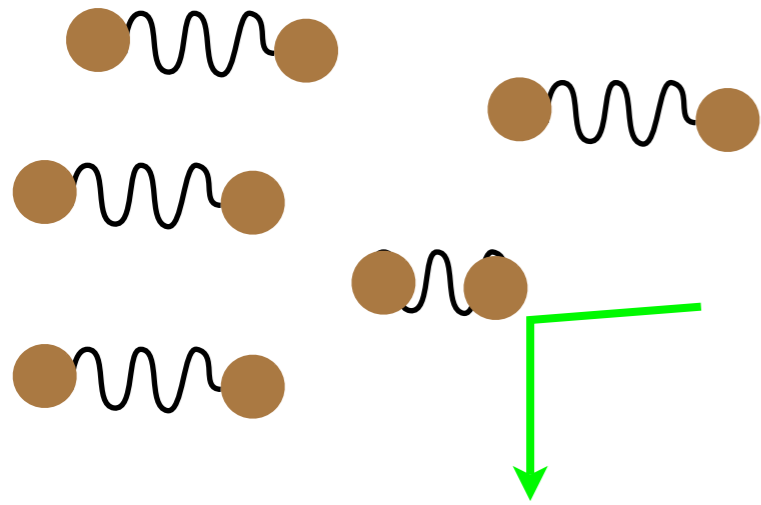


Rayleigh Scattering

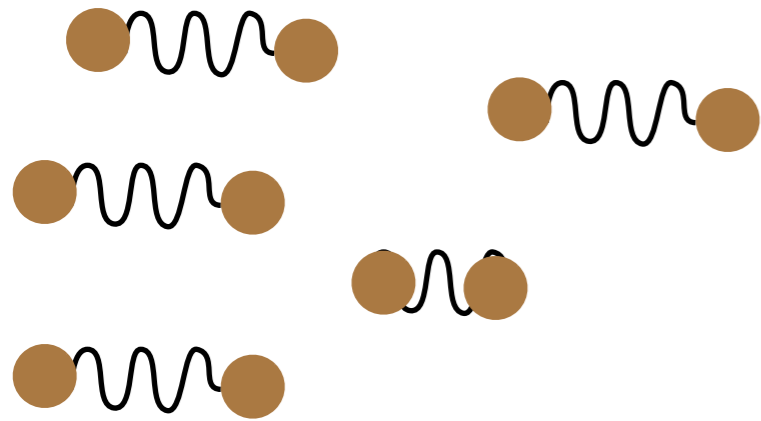
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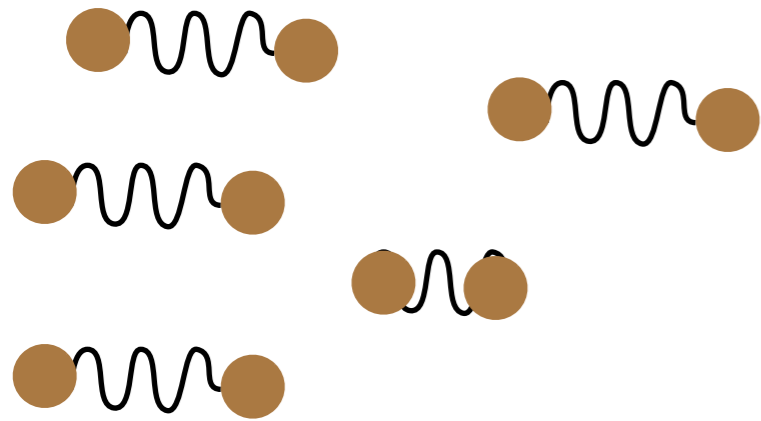


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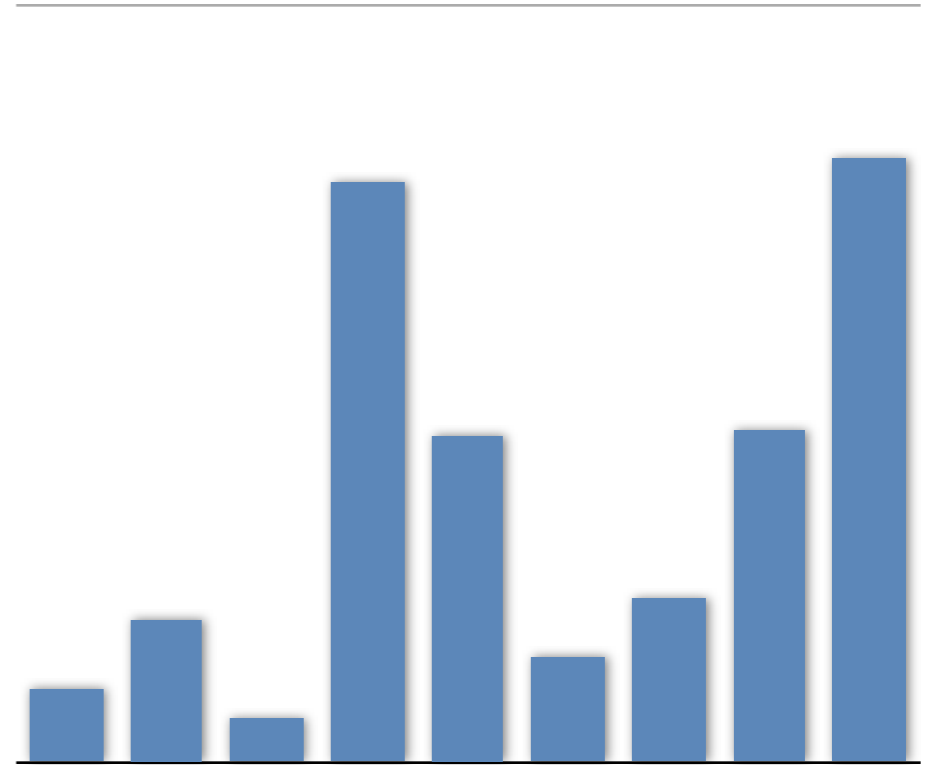
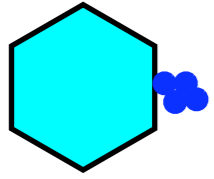


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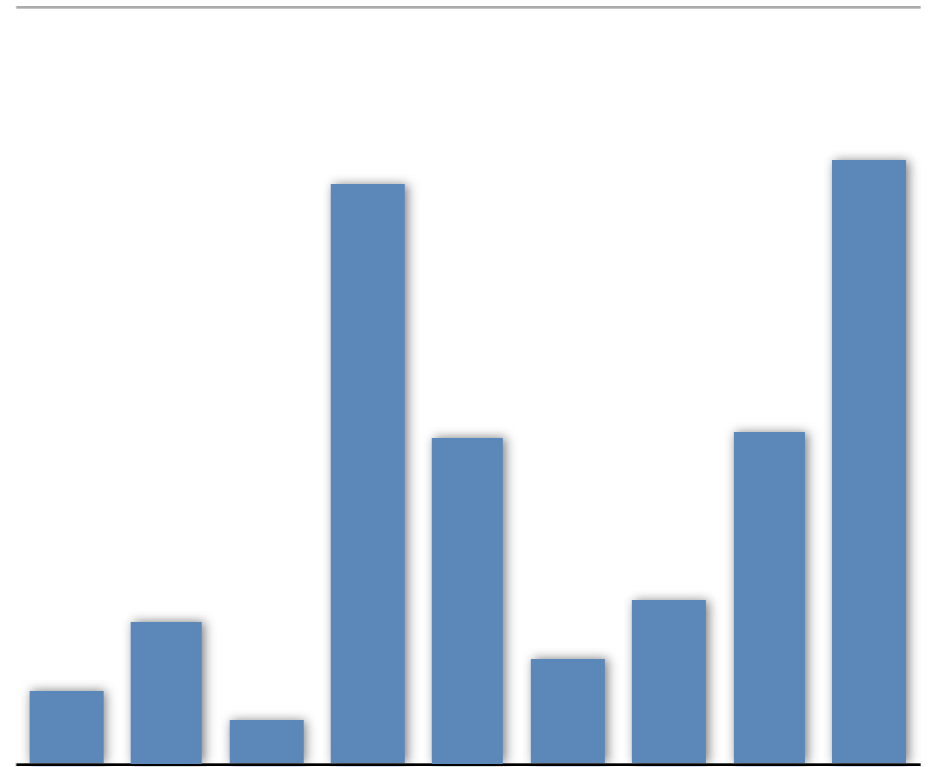
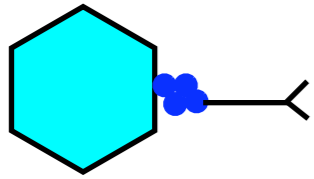


Raman Scattering

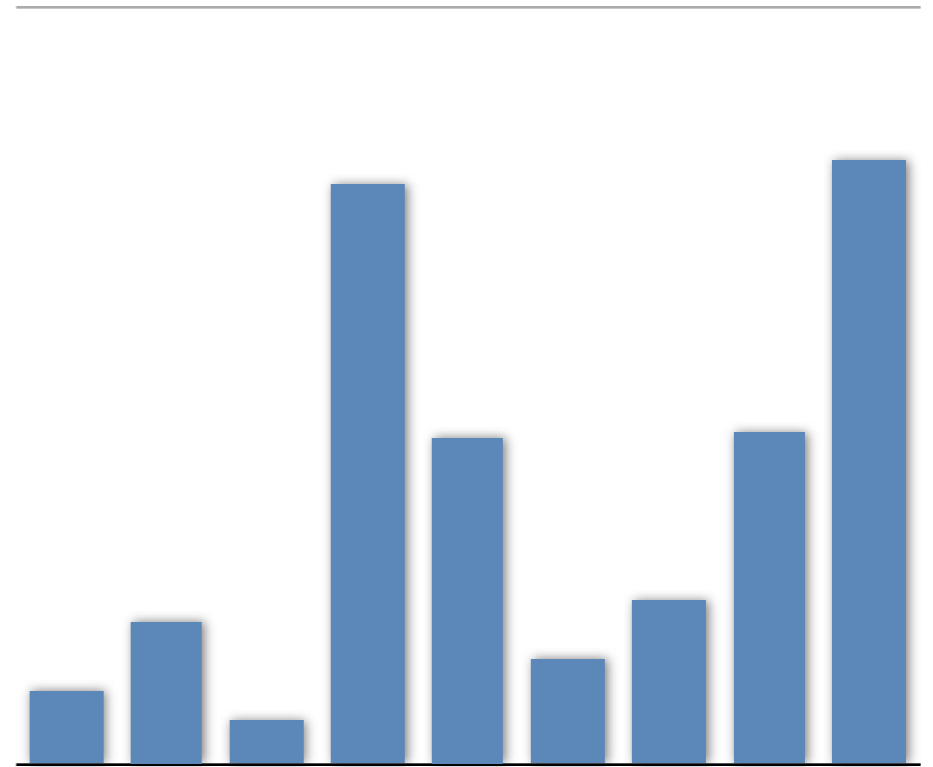
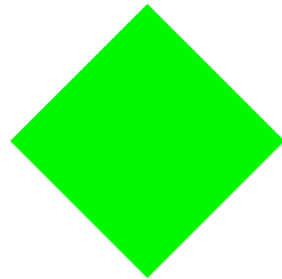
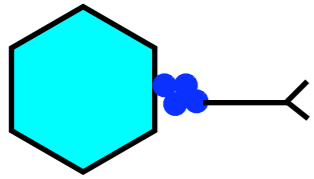
# SERRS



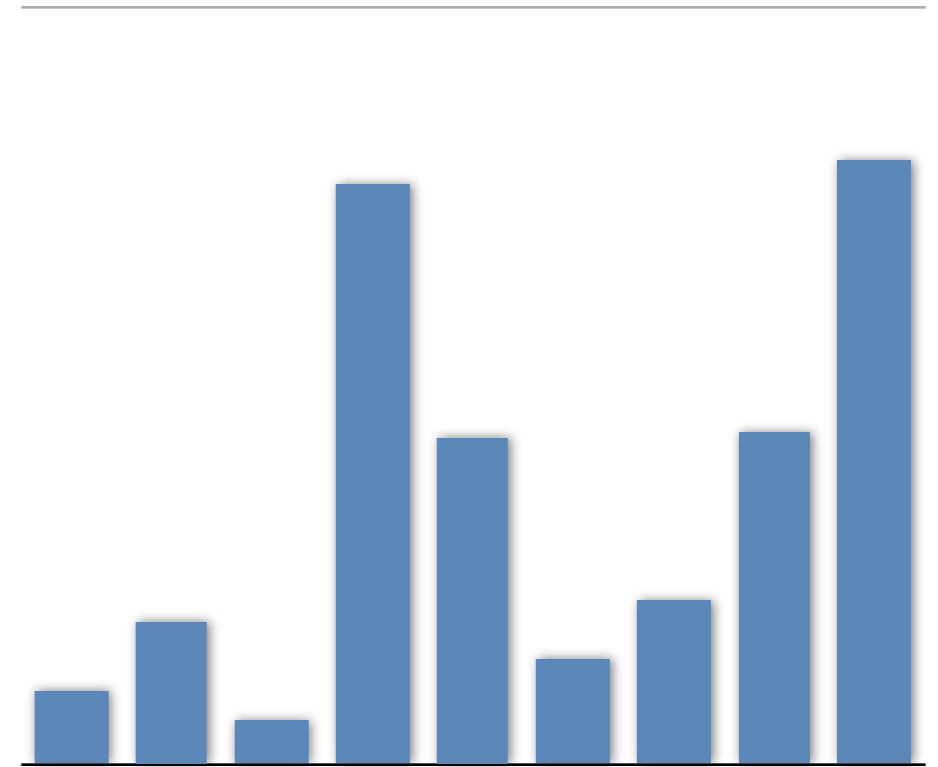
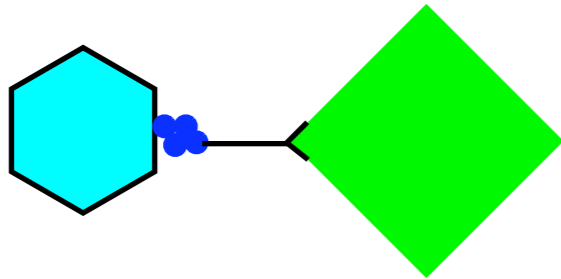
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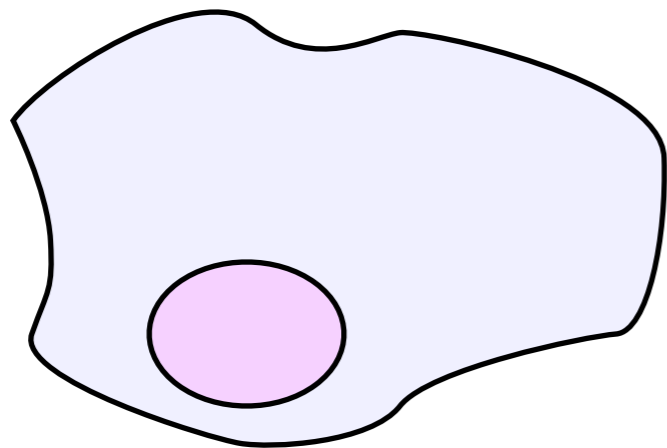
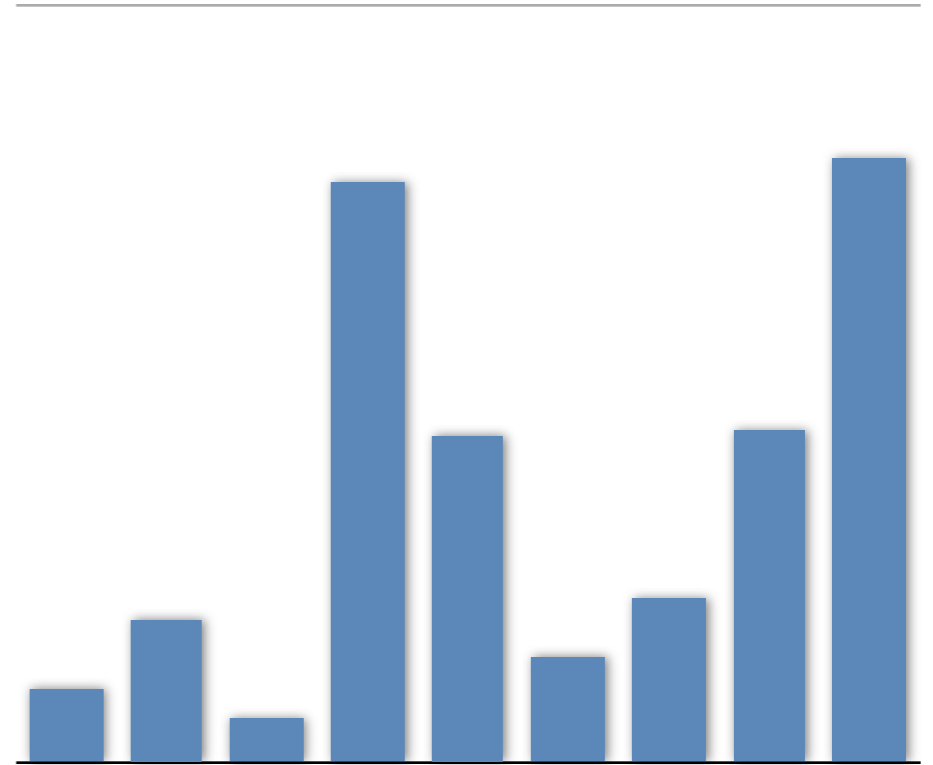
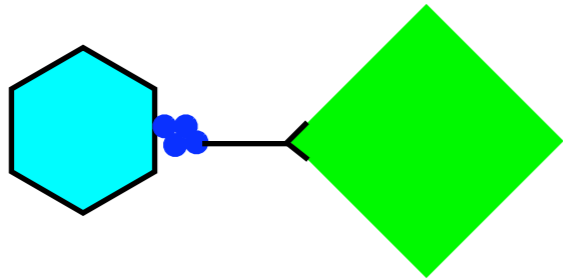
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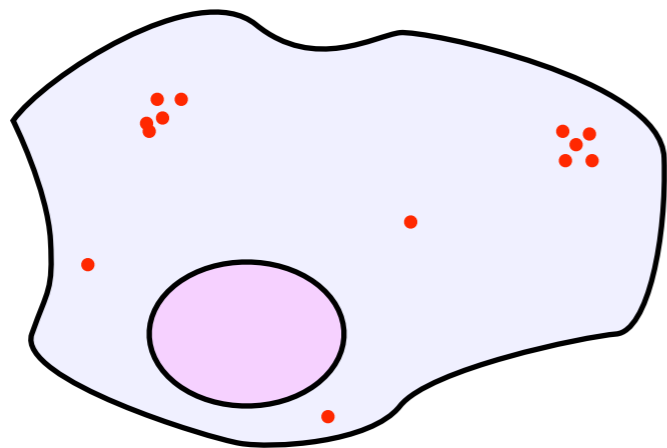
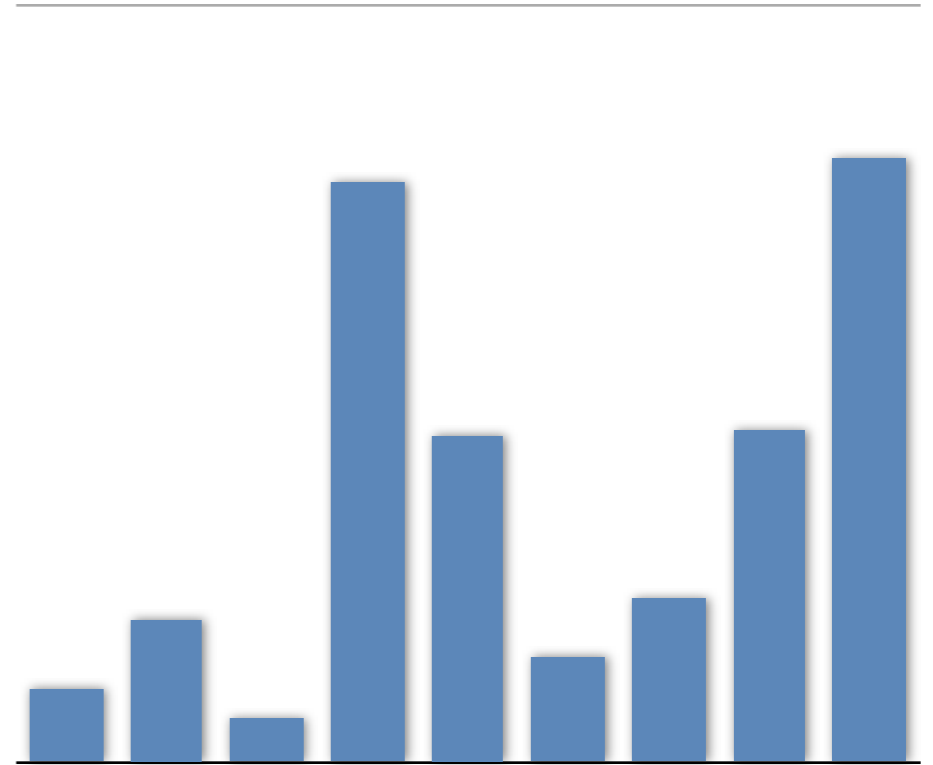
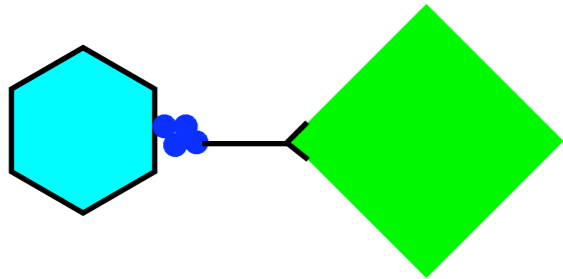
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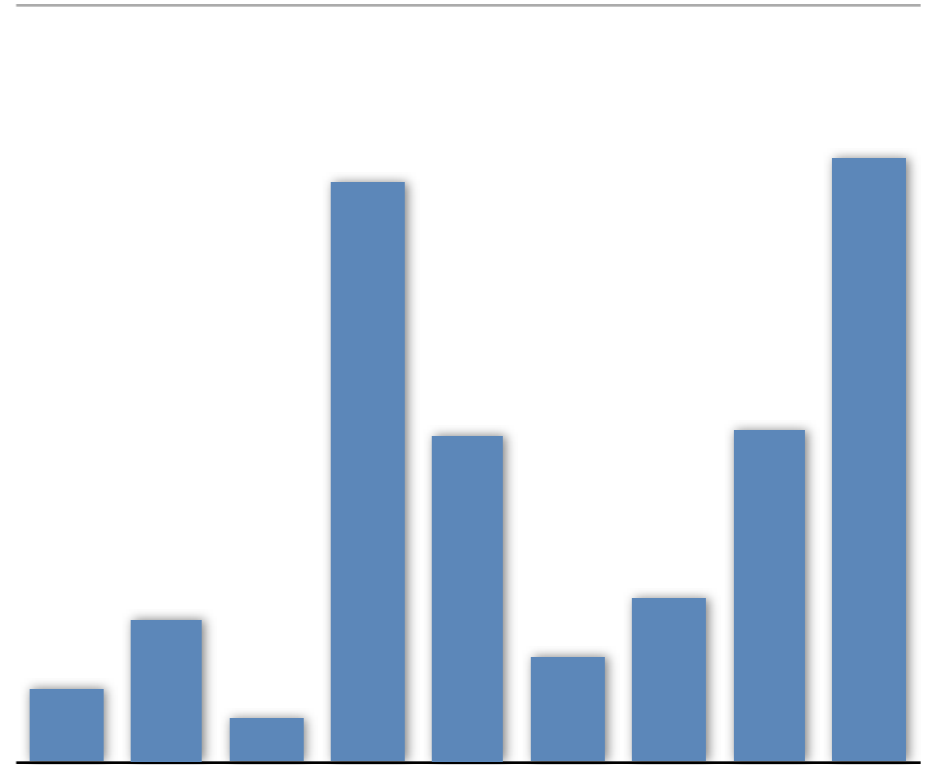
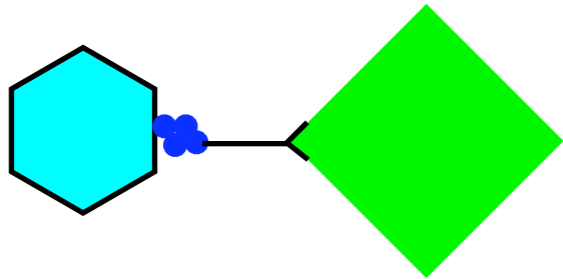
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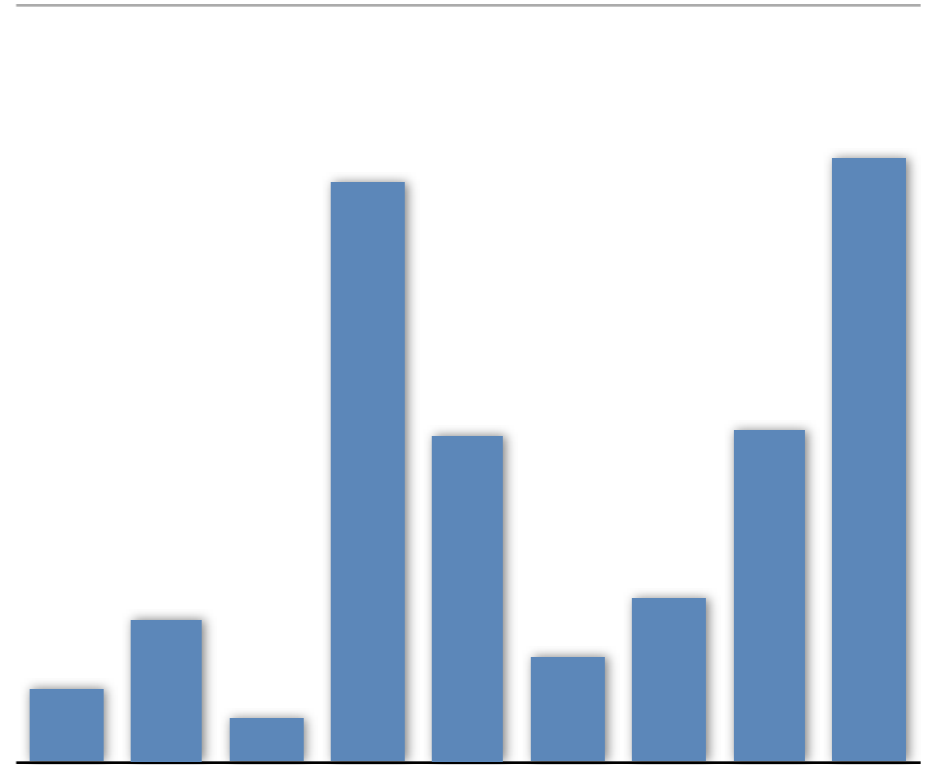
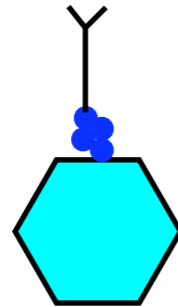
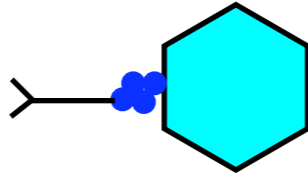
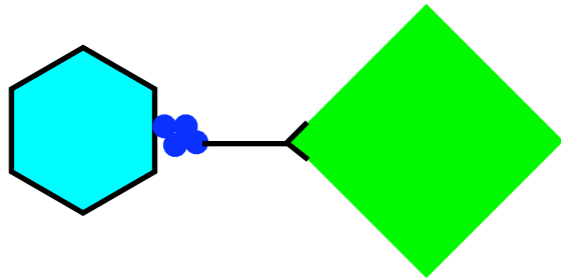


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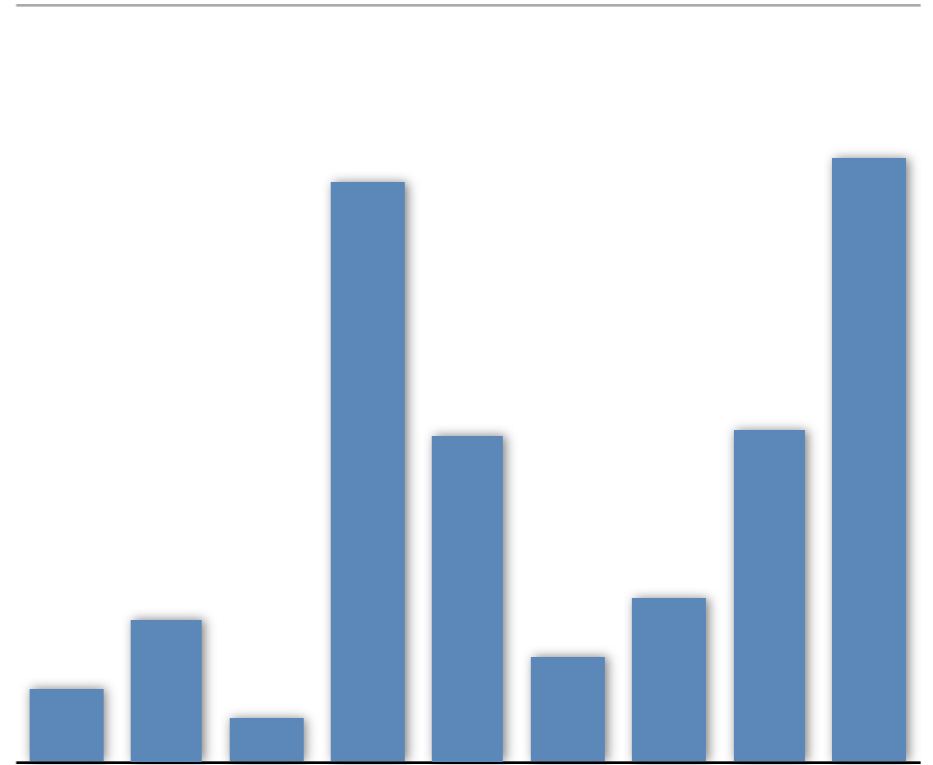
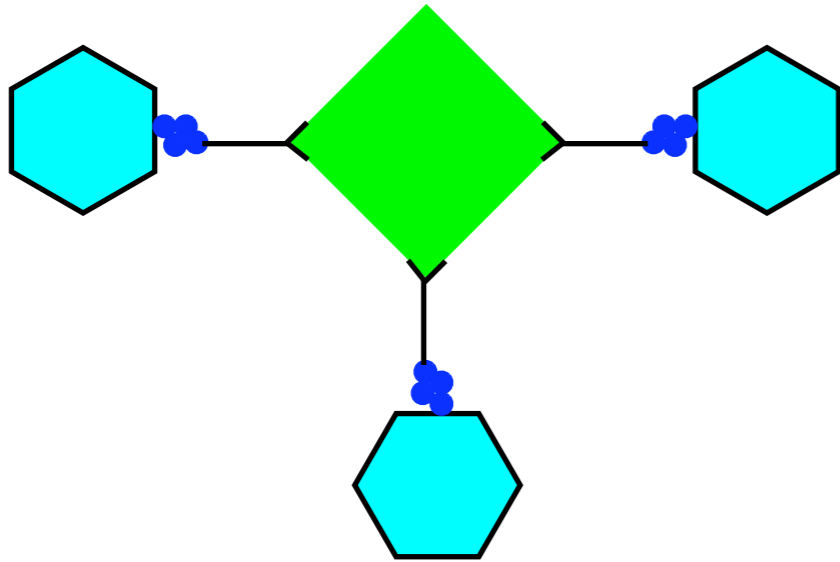




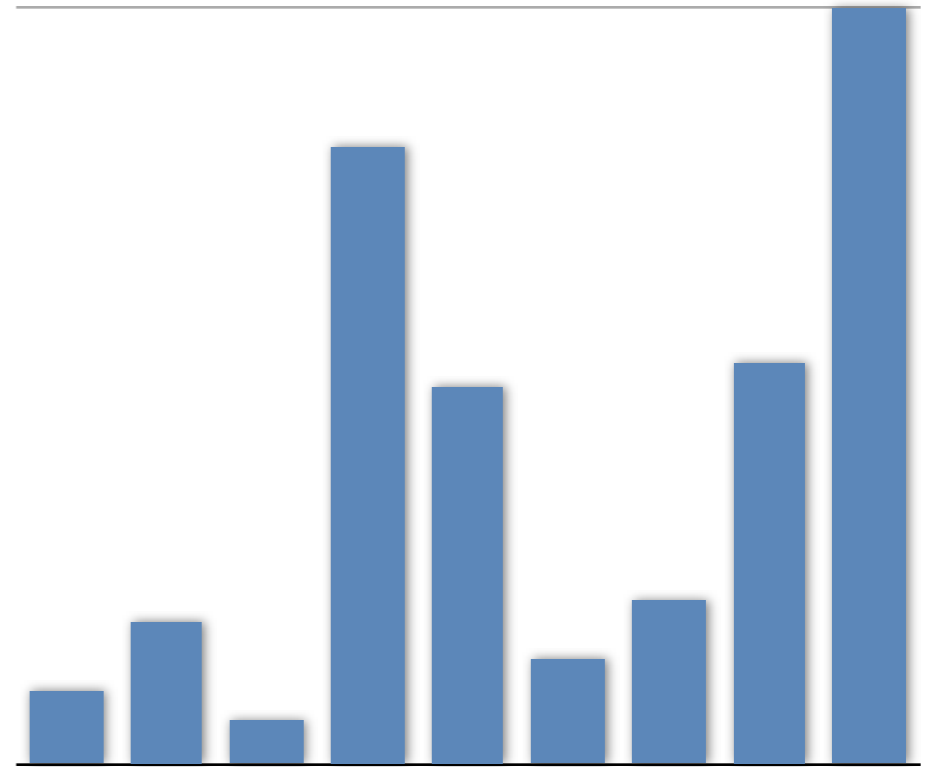
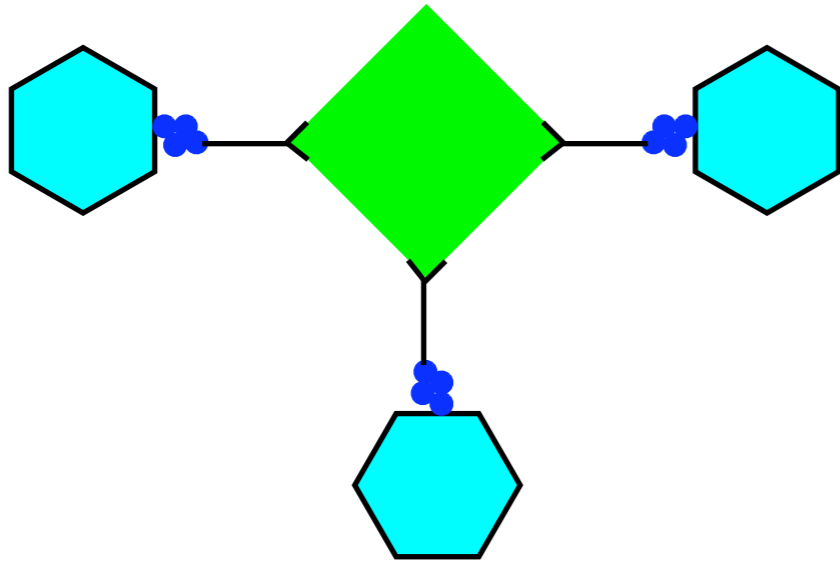
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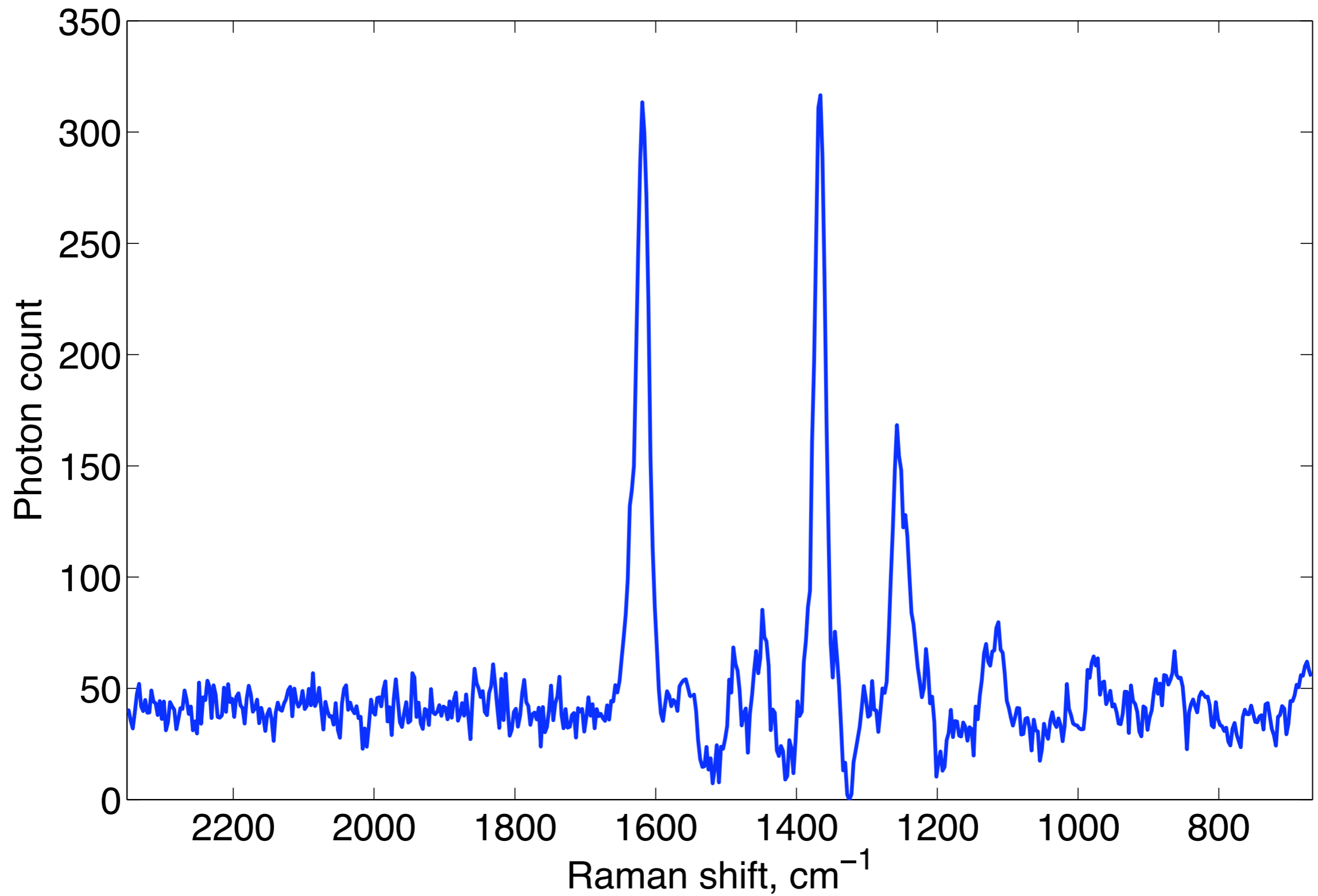
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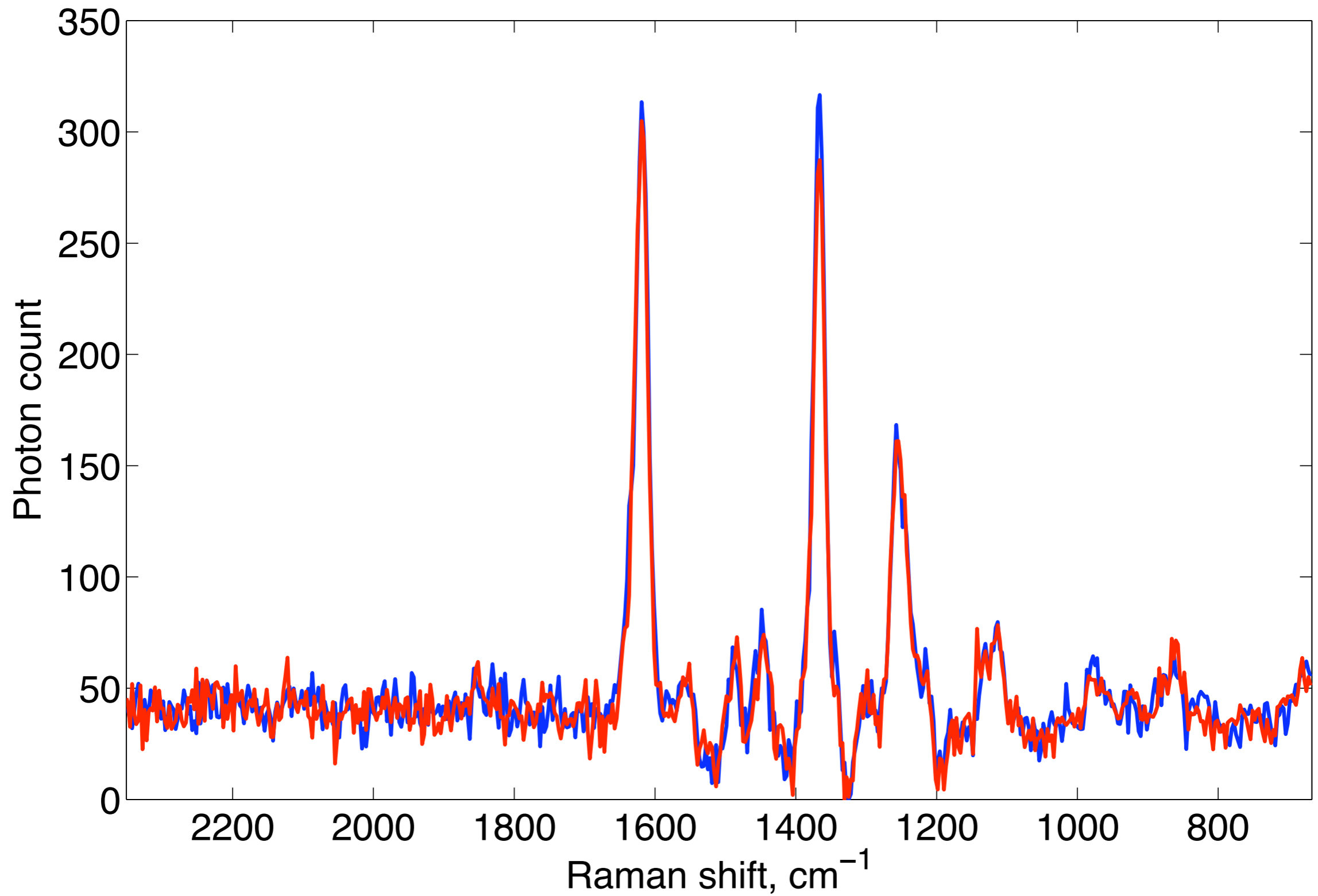
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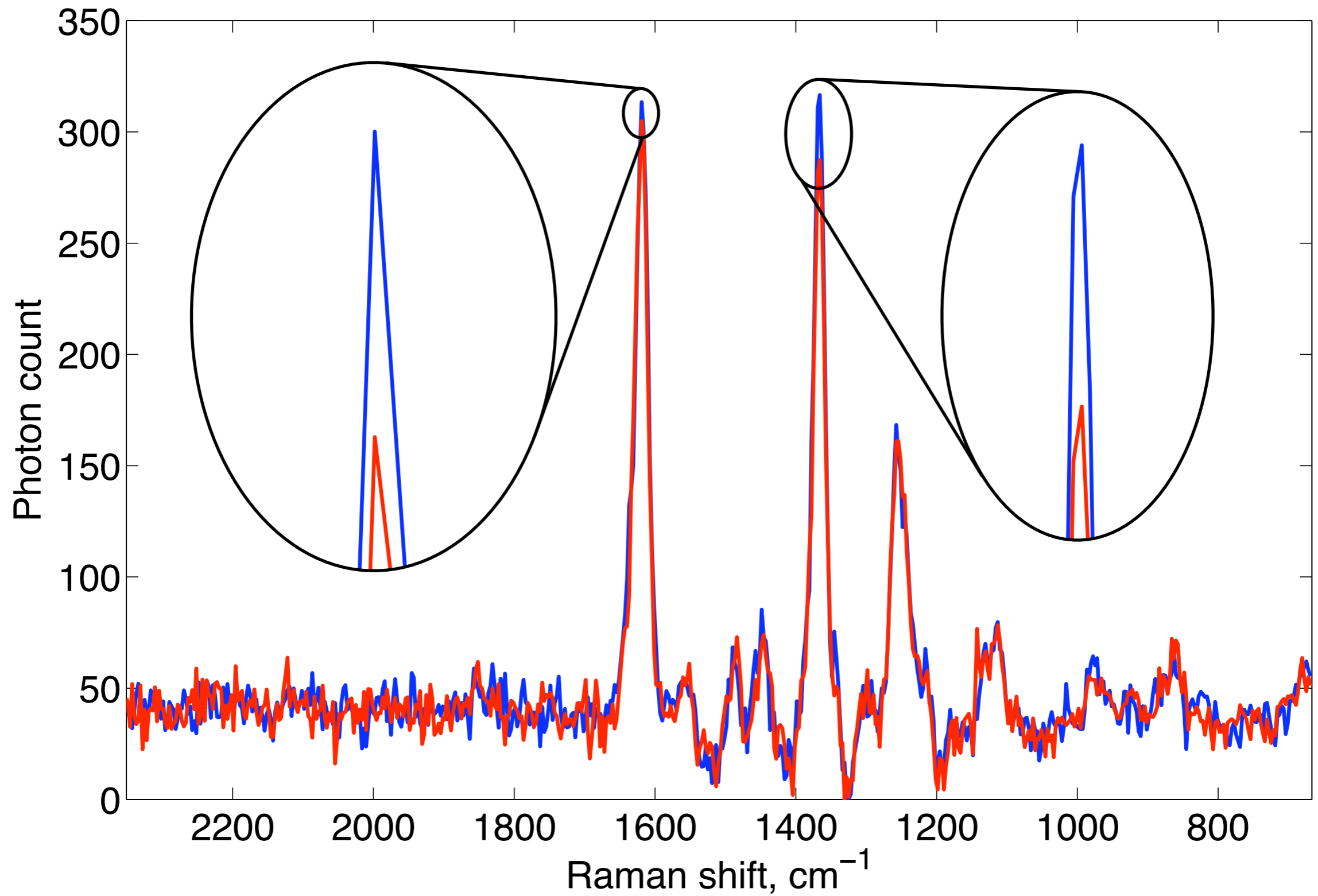
# Detecting Proteins



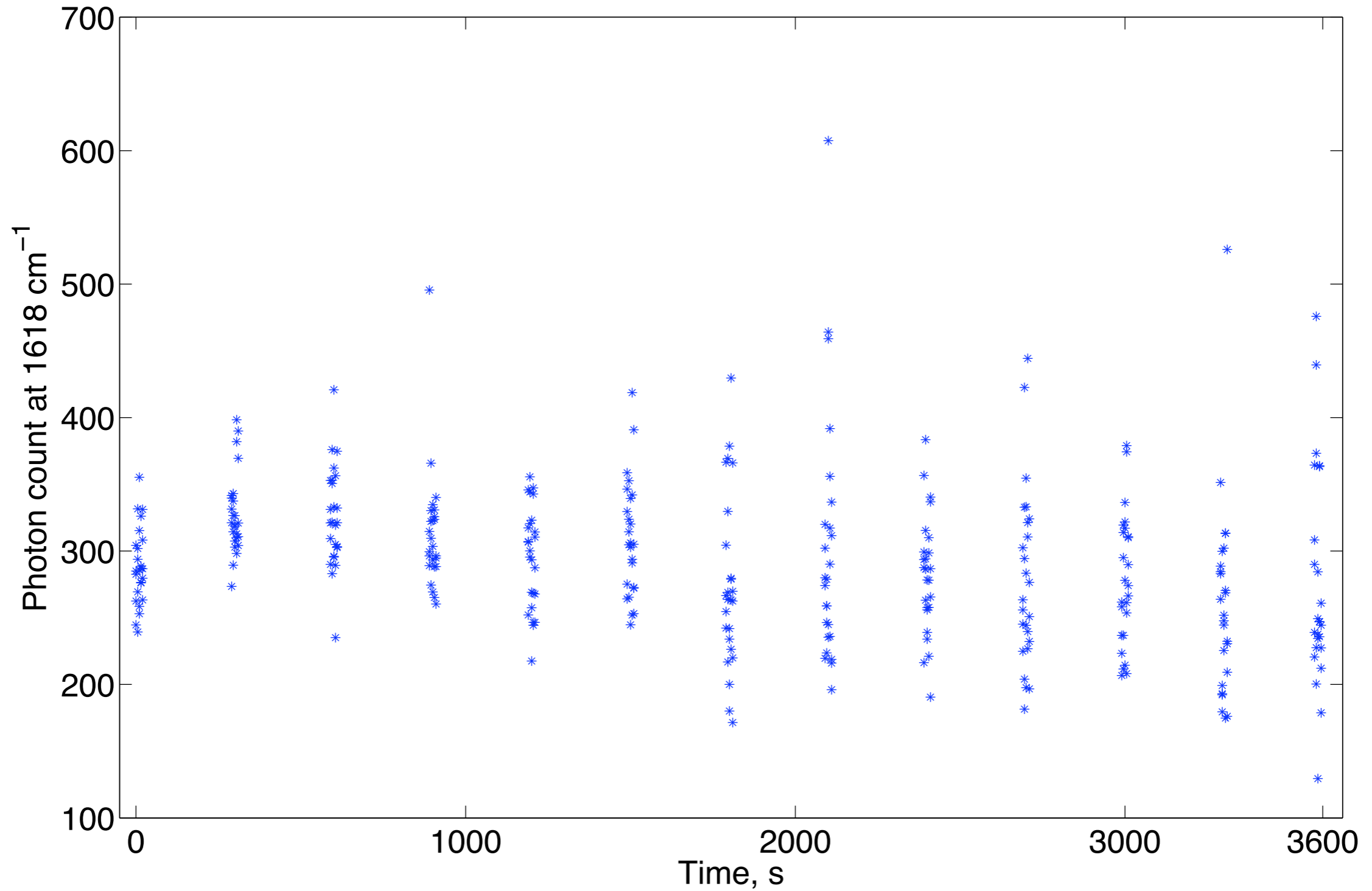
# Detecting Proteins



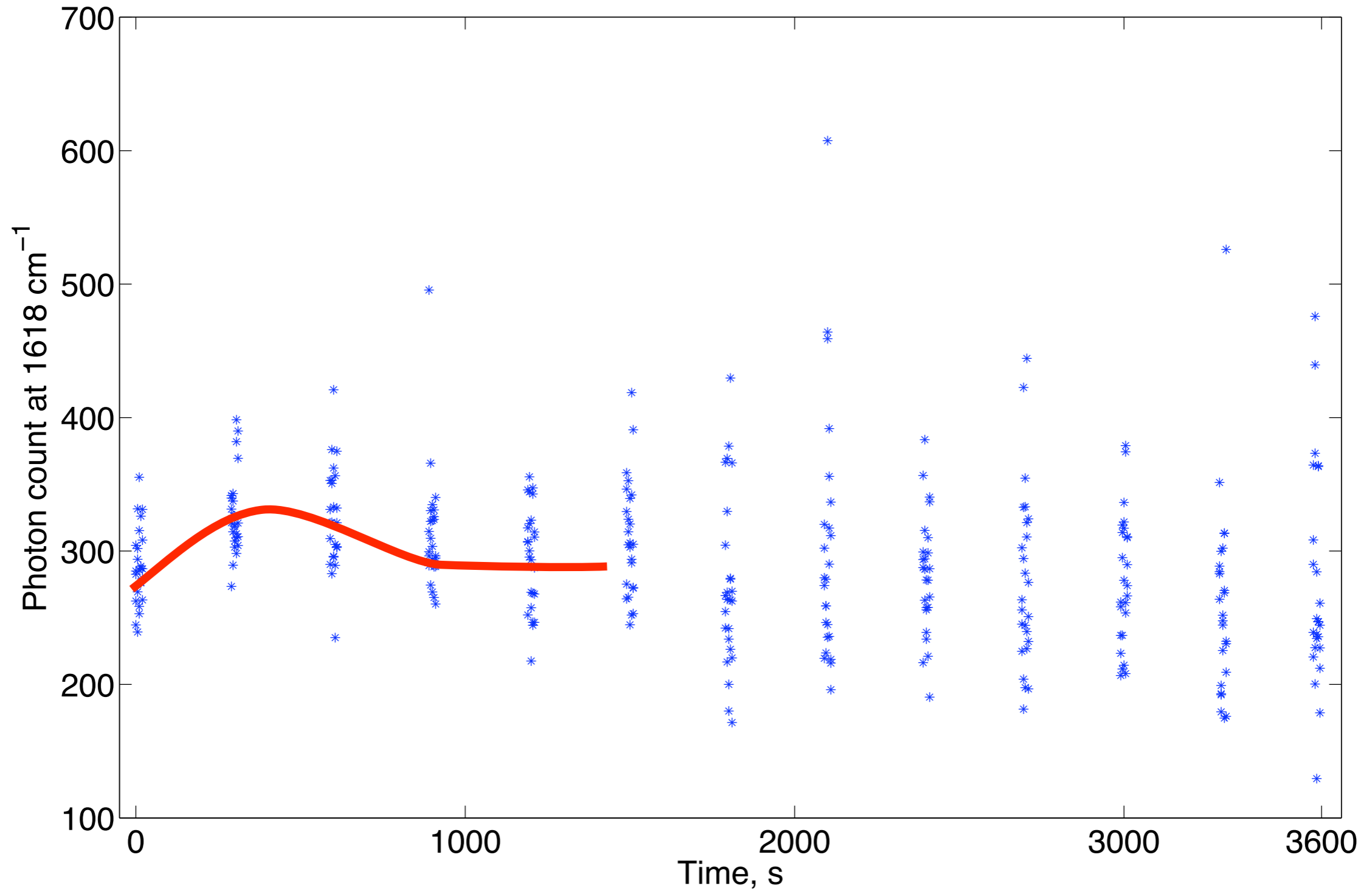
# Detecting Proteins



# Signal Changes with Time

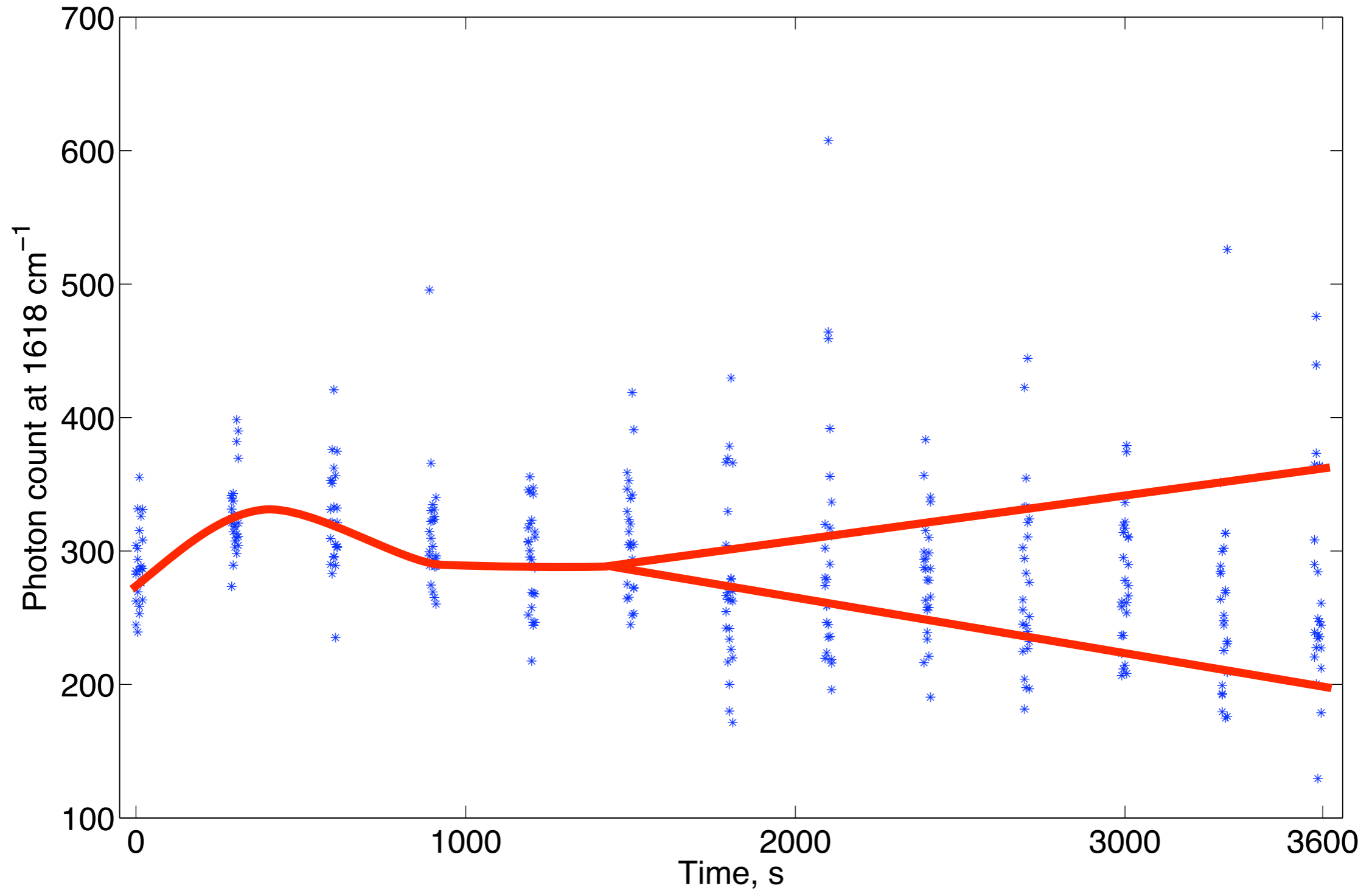


# Signal Changes with Time





# Signal Changes with Time



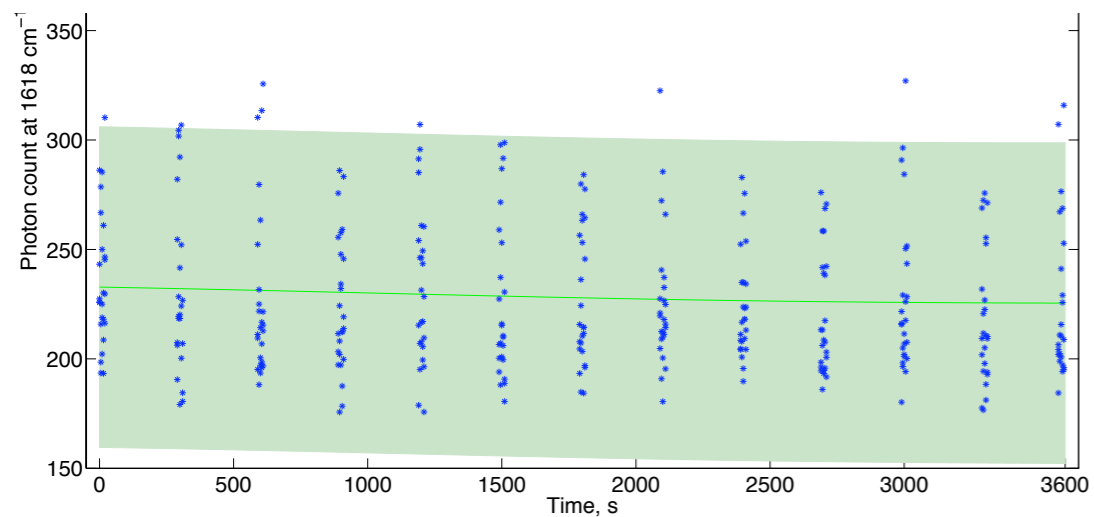
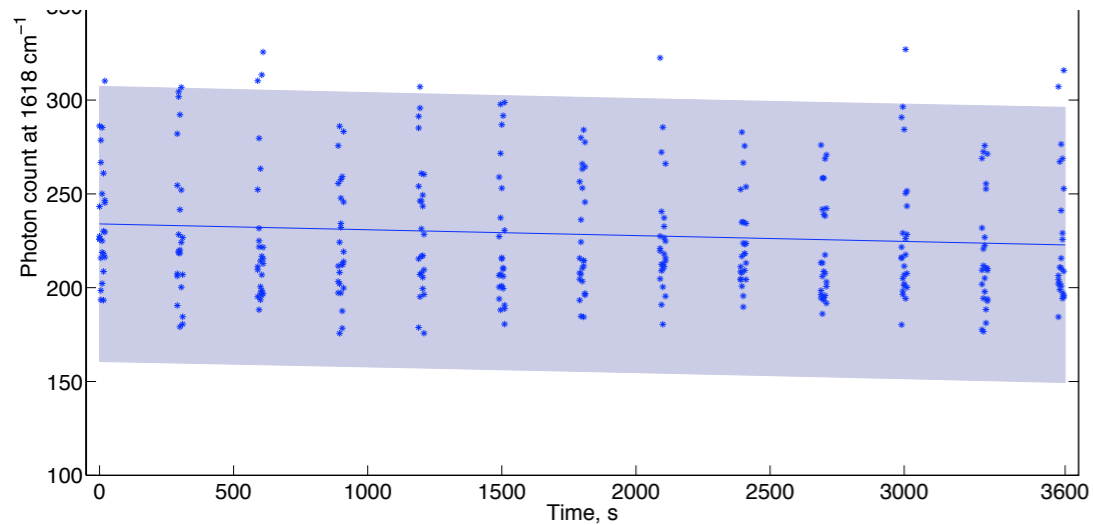
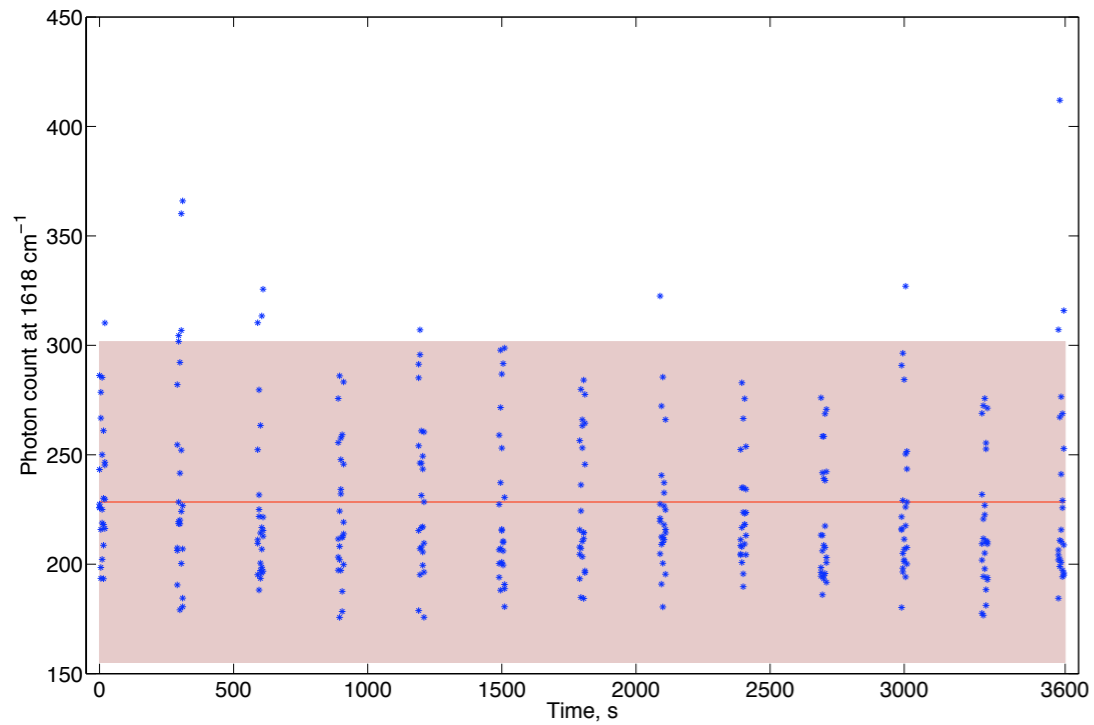
# Marginal Likelihoods are estimated with MCMC

Blank sample (no protein)

H1: 98.828%

H2: 0.003%

H3: 1.169%



# Marginal Likelihoods are estimated with MCMC

Blank sample (no protein)

H1: 98.828%

H2: 0.003%

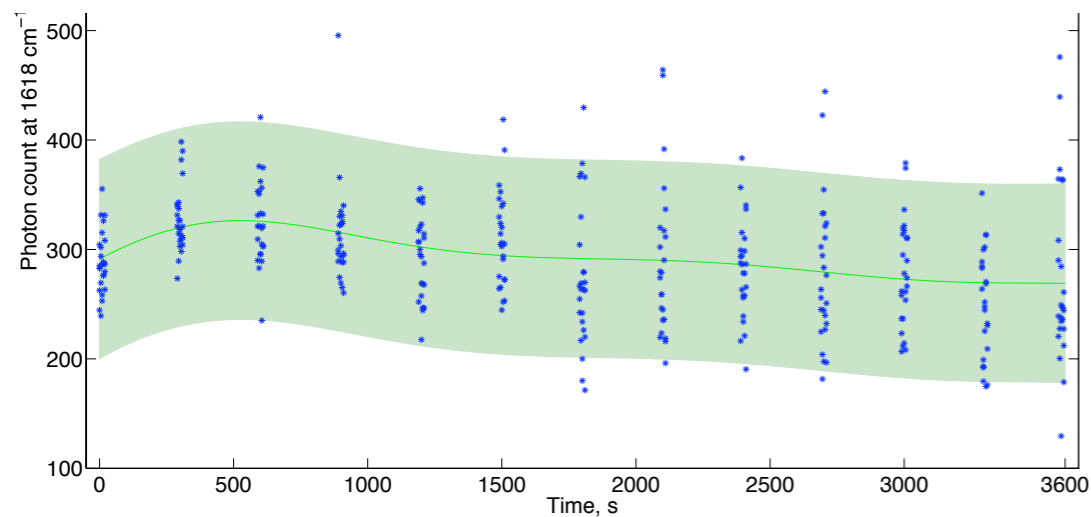
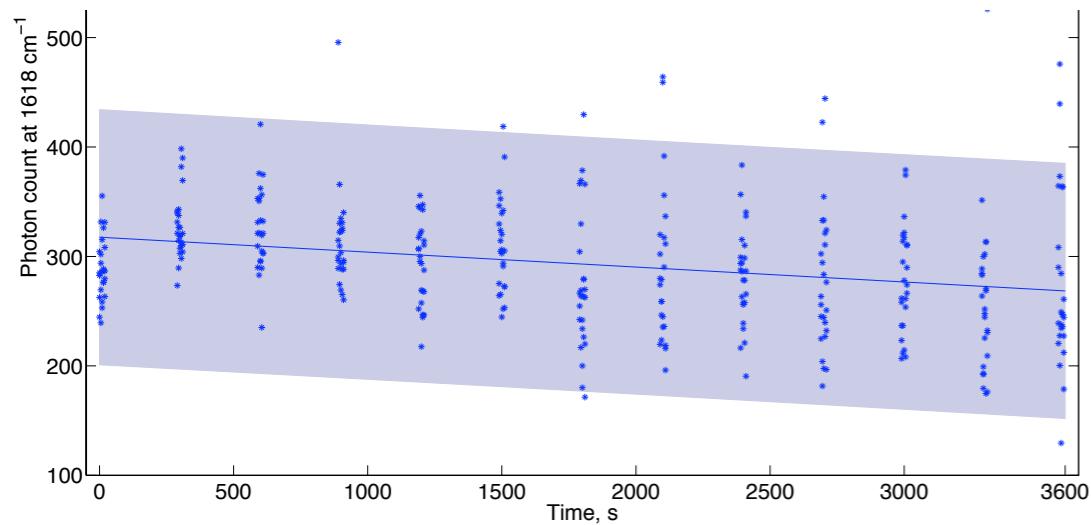
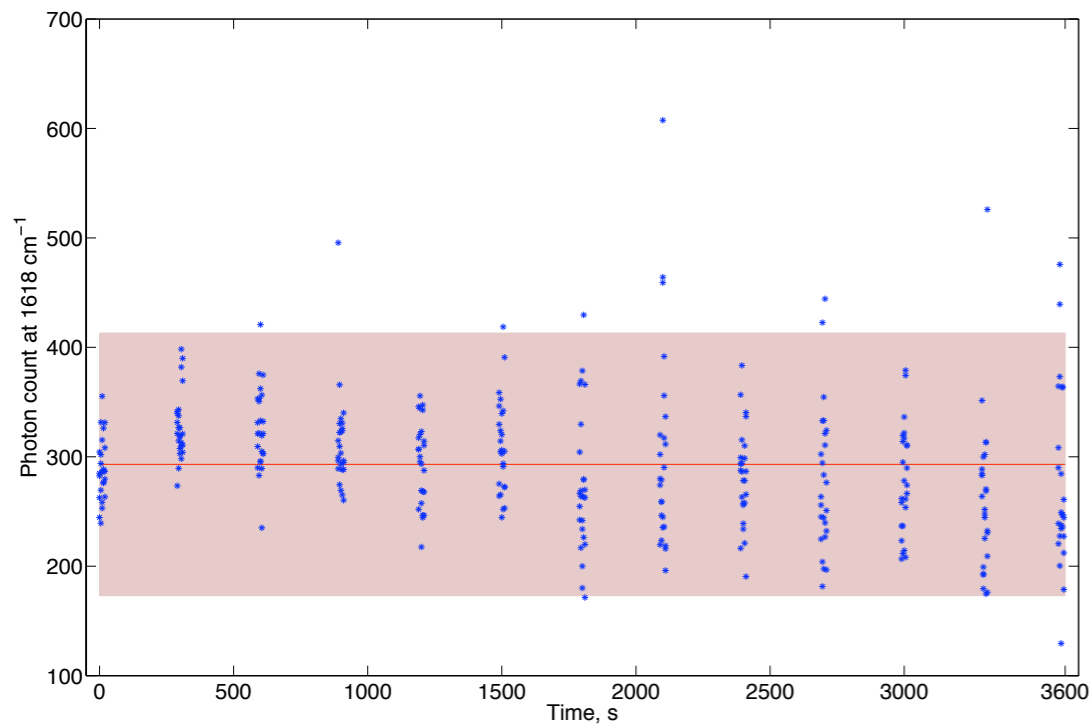
H3: 1.169%

Target protein is present

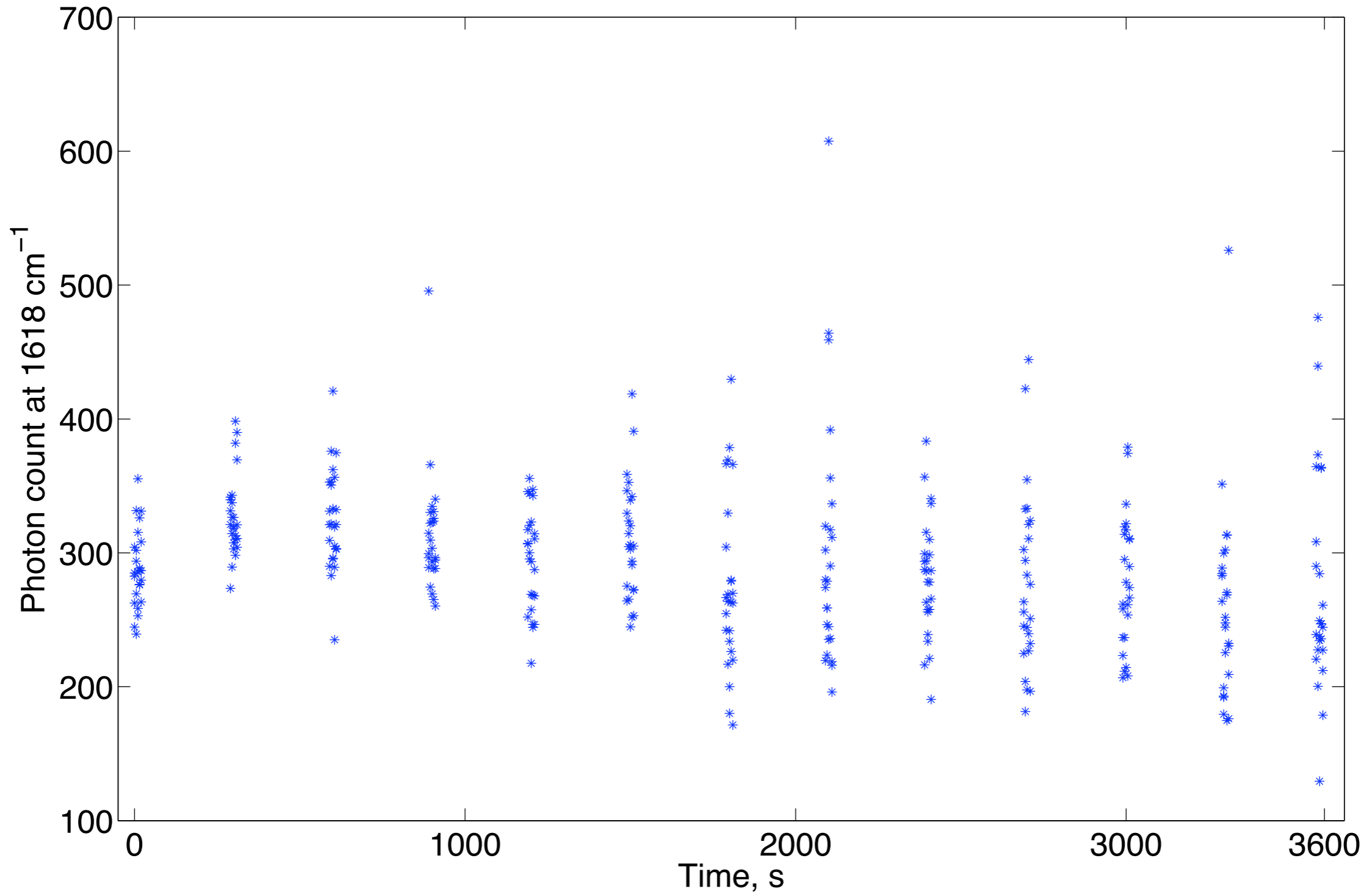
H1: 0.301%

H2: 0.101%

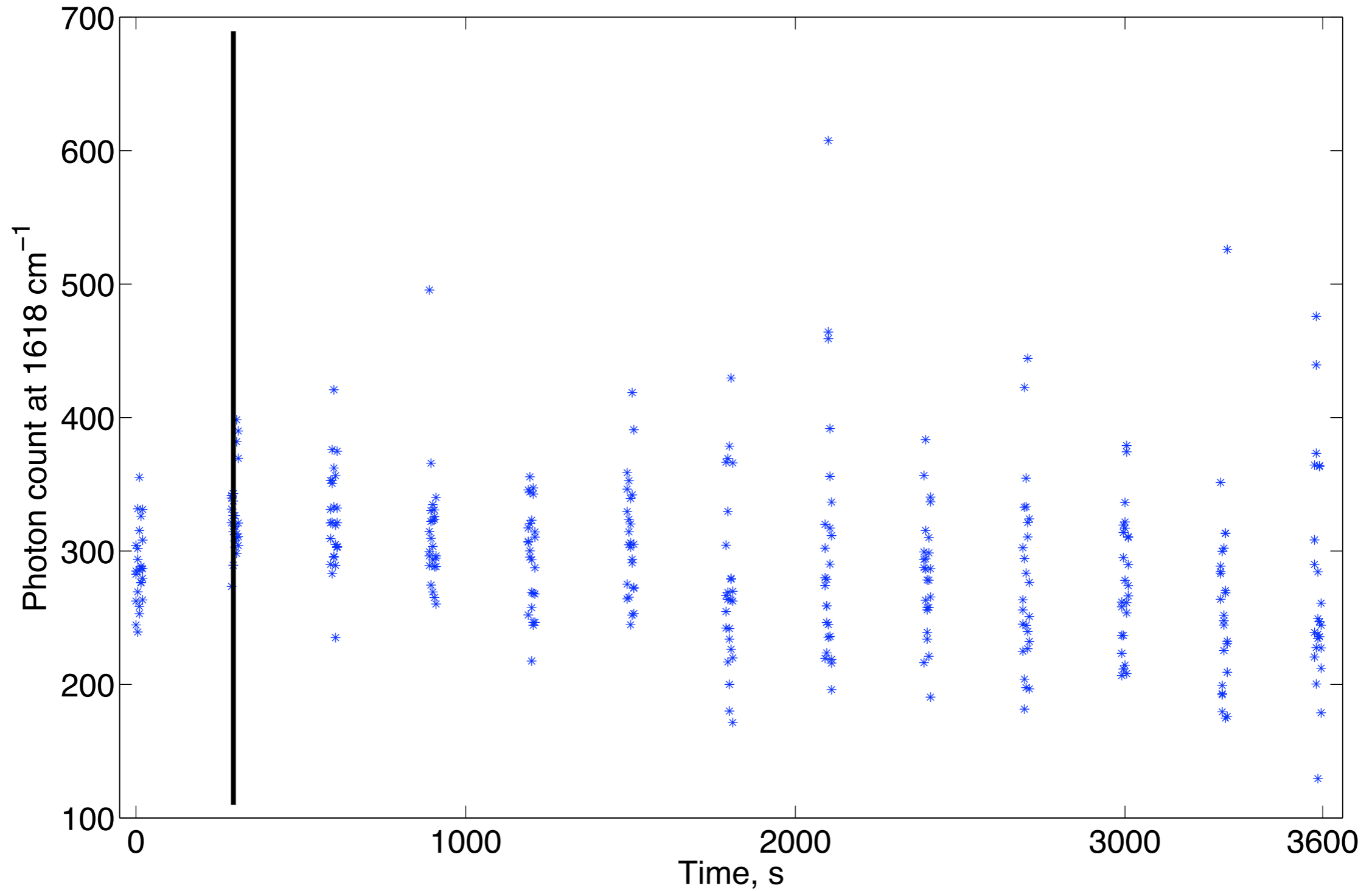
H3: 99.598%



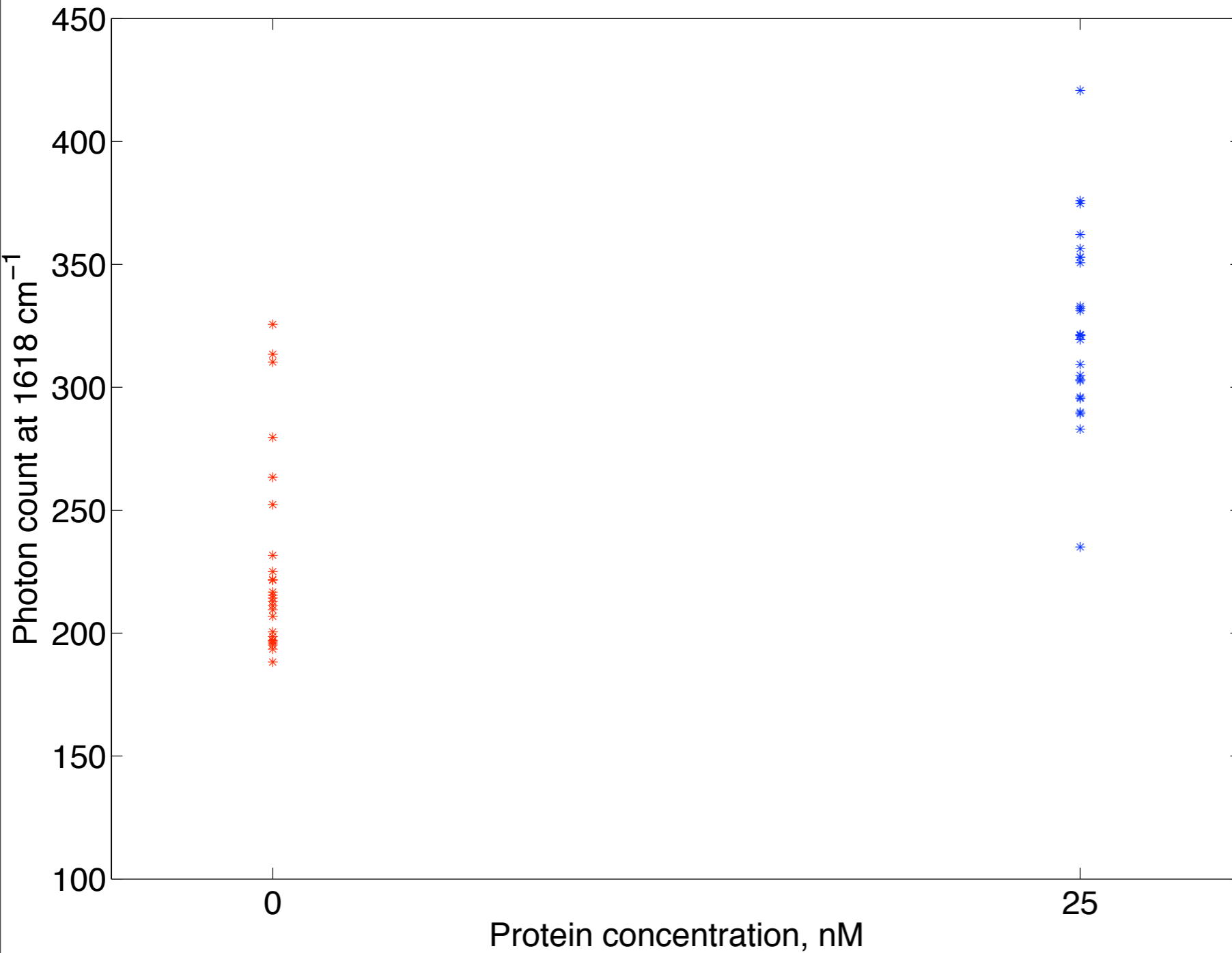
# Signal Changes with Time



# Signal Changes with Time



# Is there a difference?



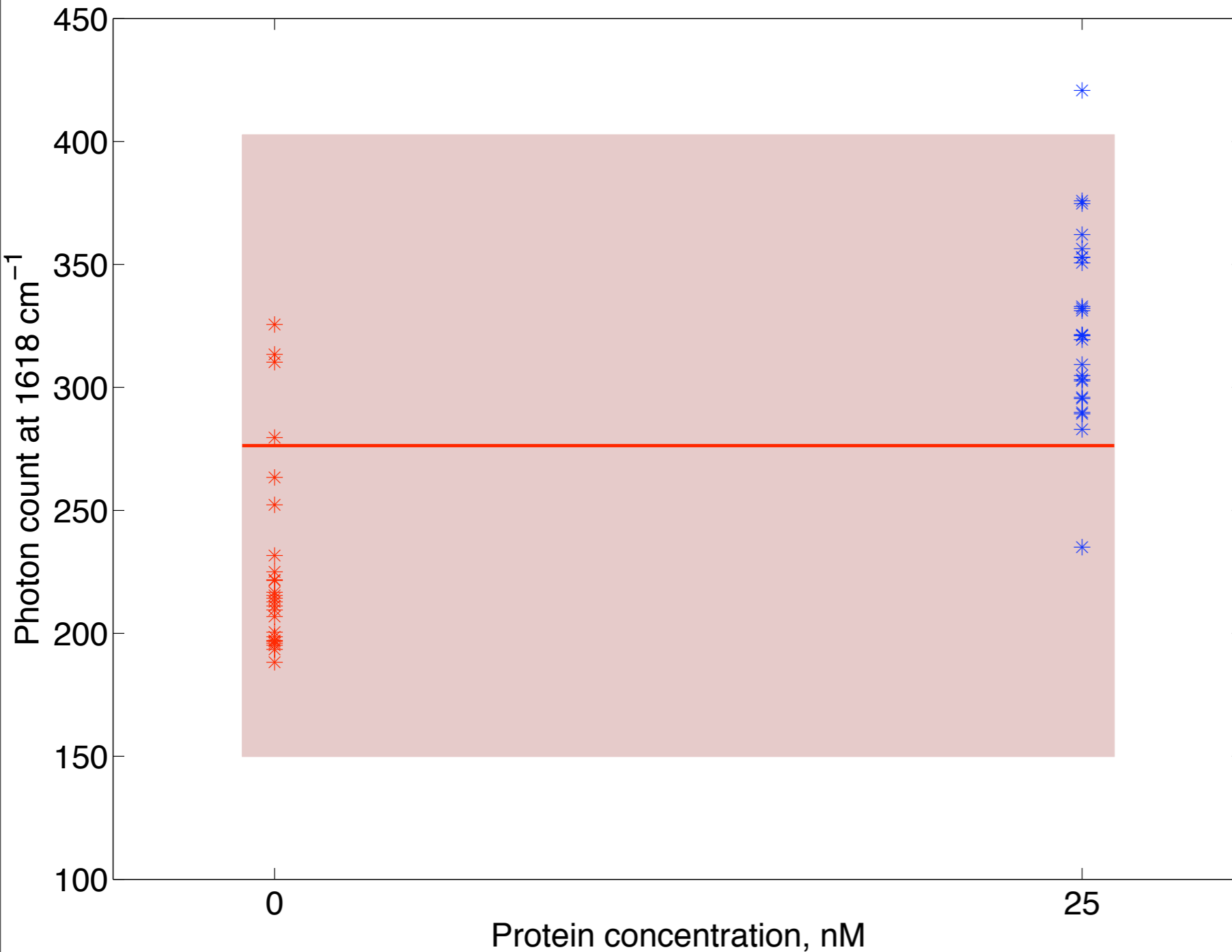
**Wilcoxon–Mann–Whitney:**

median: 214

median: 321

P = 9.5×10<sup>-8</sup>

# Is there a difference?



## Wilcoxon–Mann–Whitney:

median: 214

median: 321

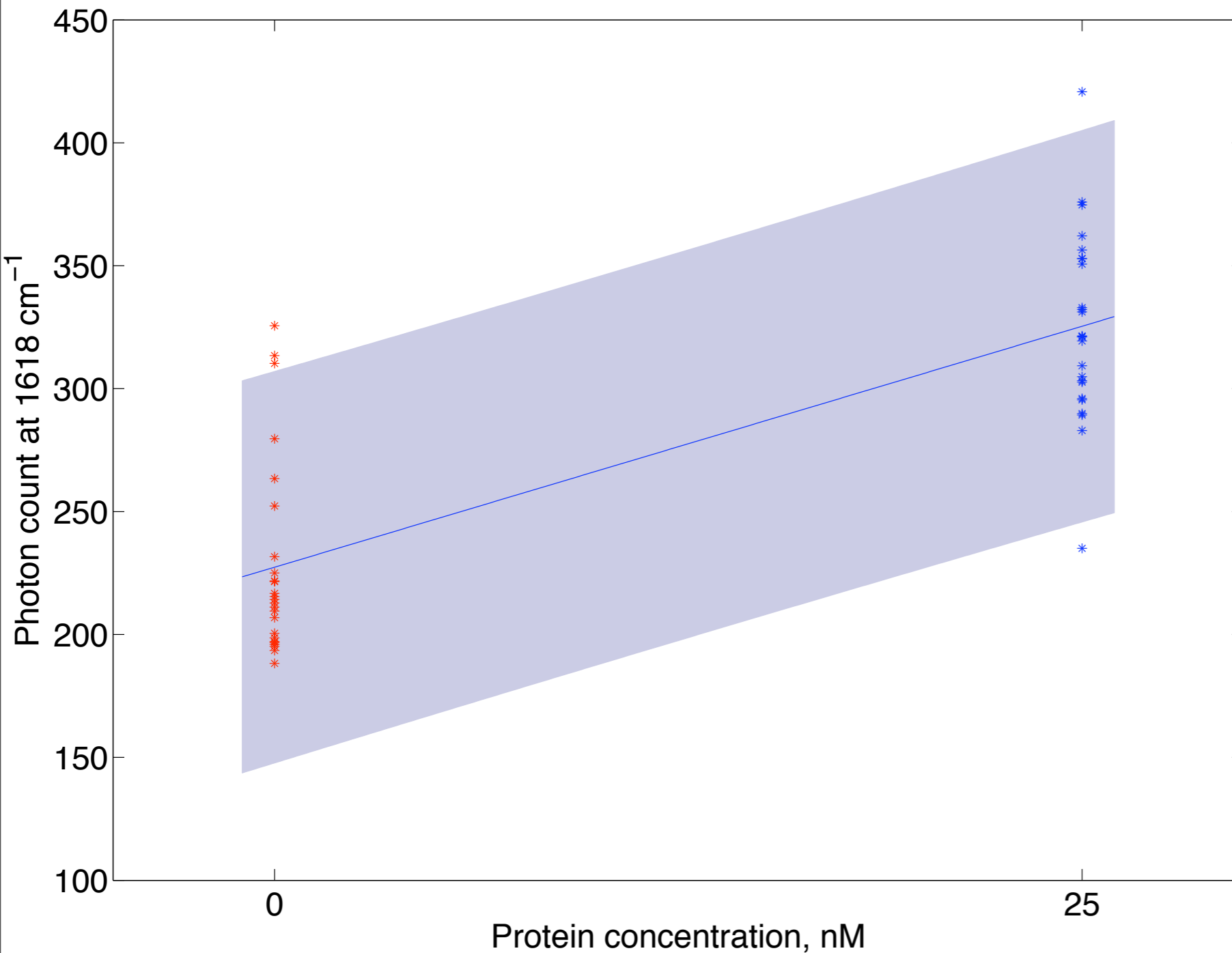
$P = 9.5 \times 10^{-8}$

## Bayesian hypotheses testing:

Constant:

Linear:

# Is there a difference?



## Wilcoxon–Mann–Whitney:

median: 214

median: 321

P =  $9.5 \times 10^{-8}$

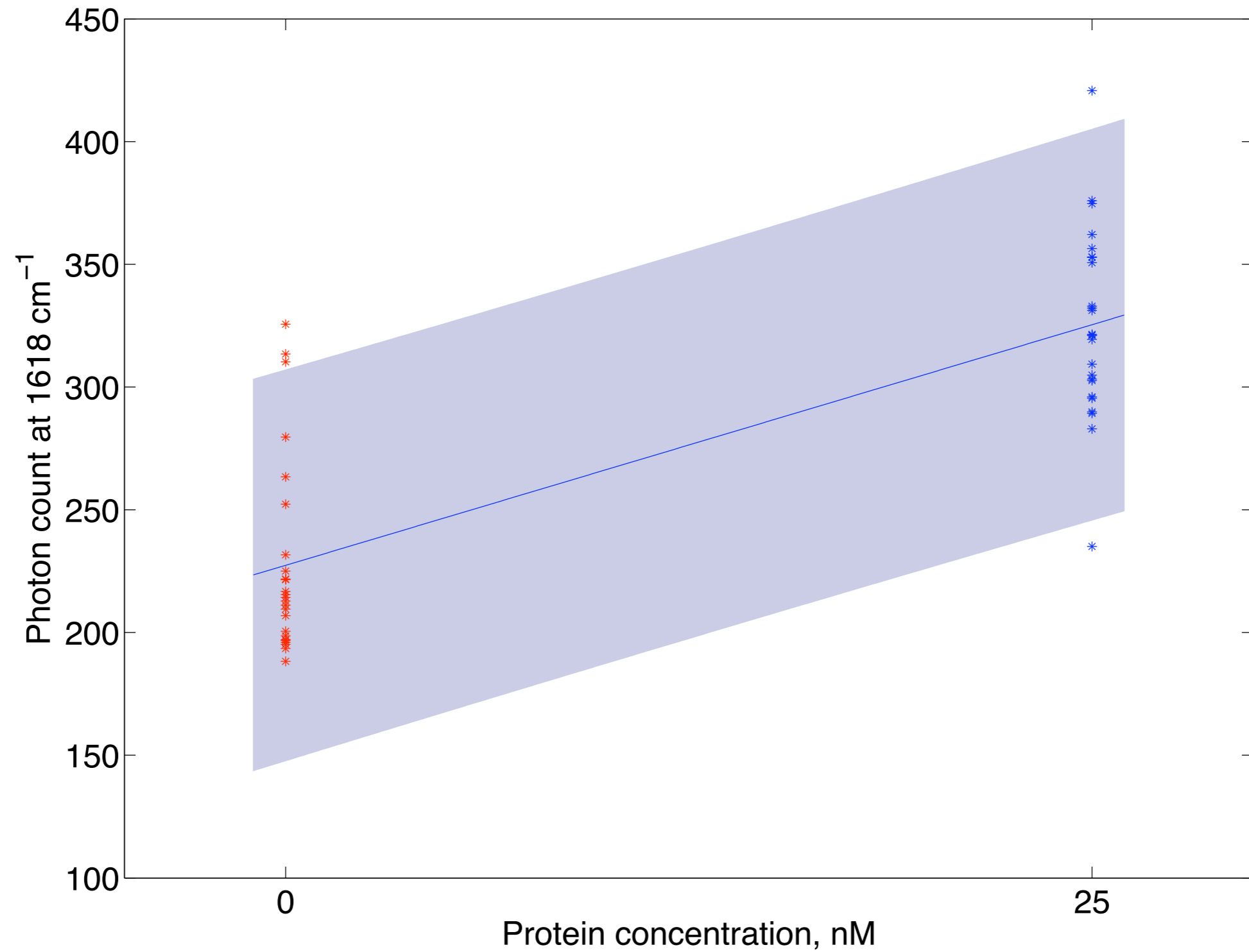
## Bayesian hypotheses testing:

Constant:  $3 \times 10^{-6}$  %

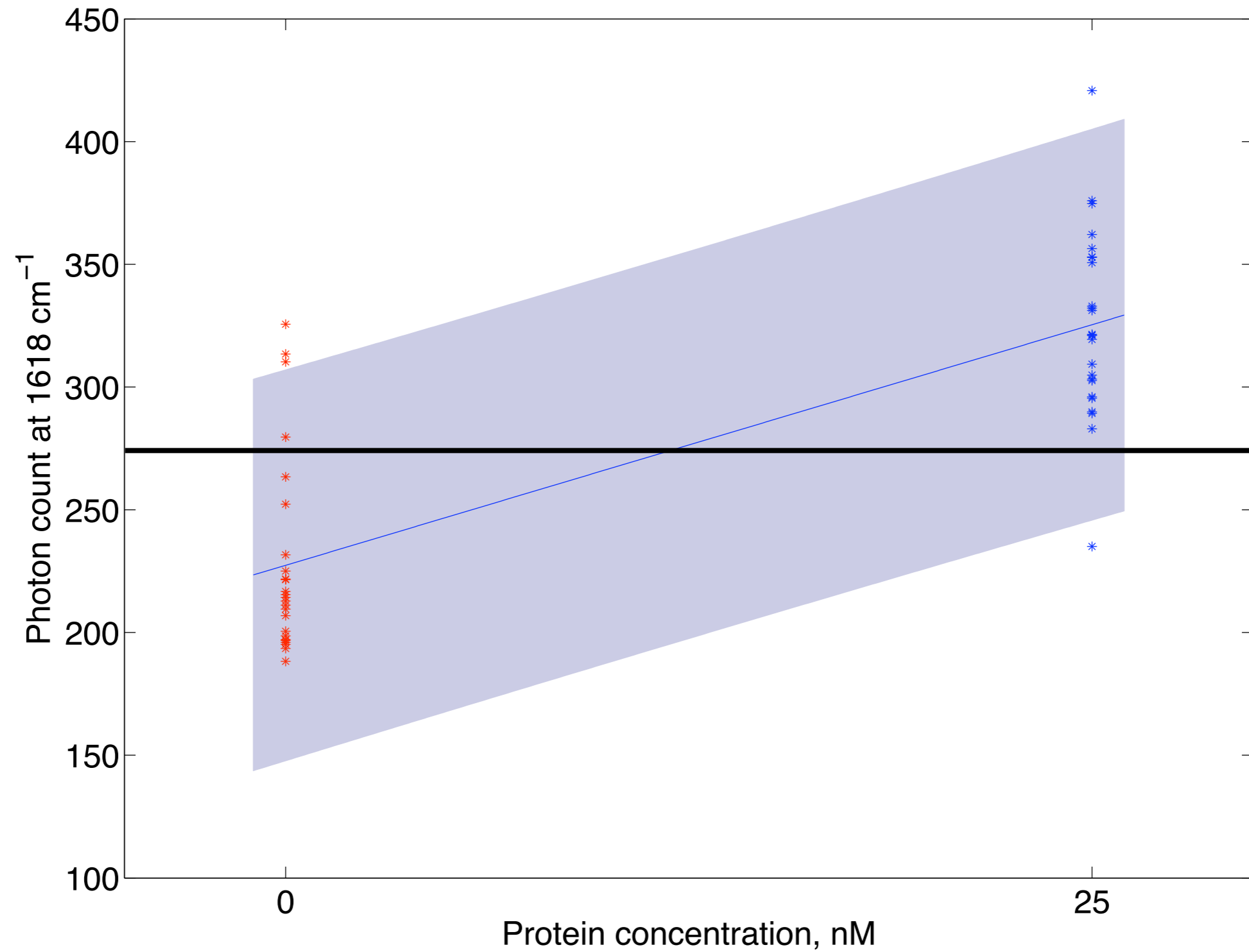
Linear: 99.99999 %



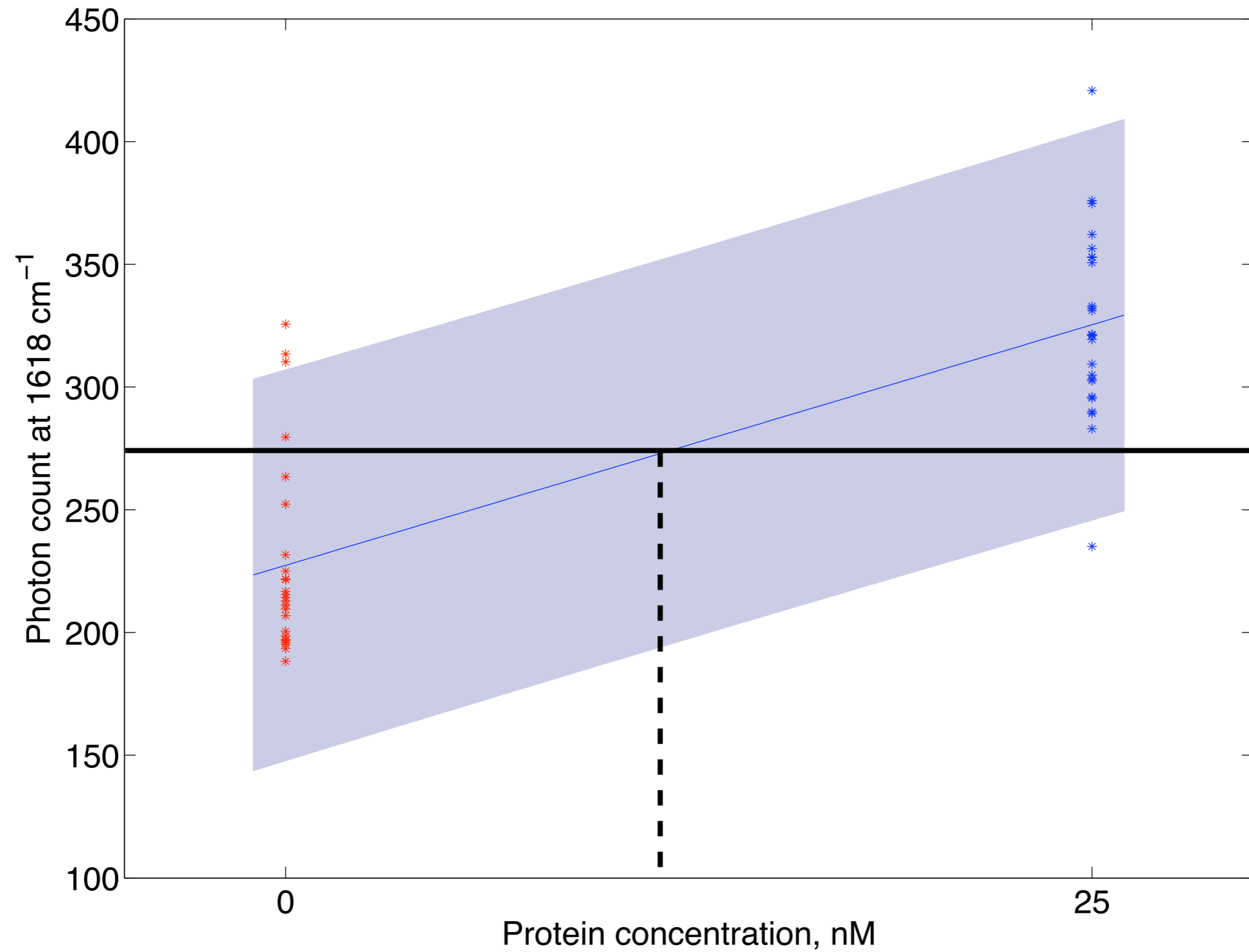
# Can we perform regression?



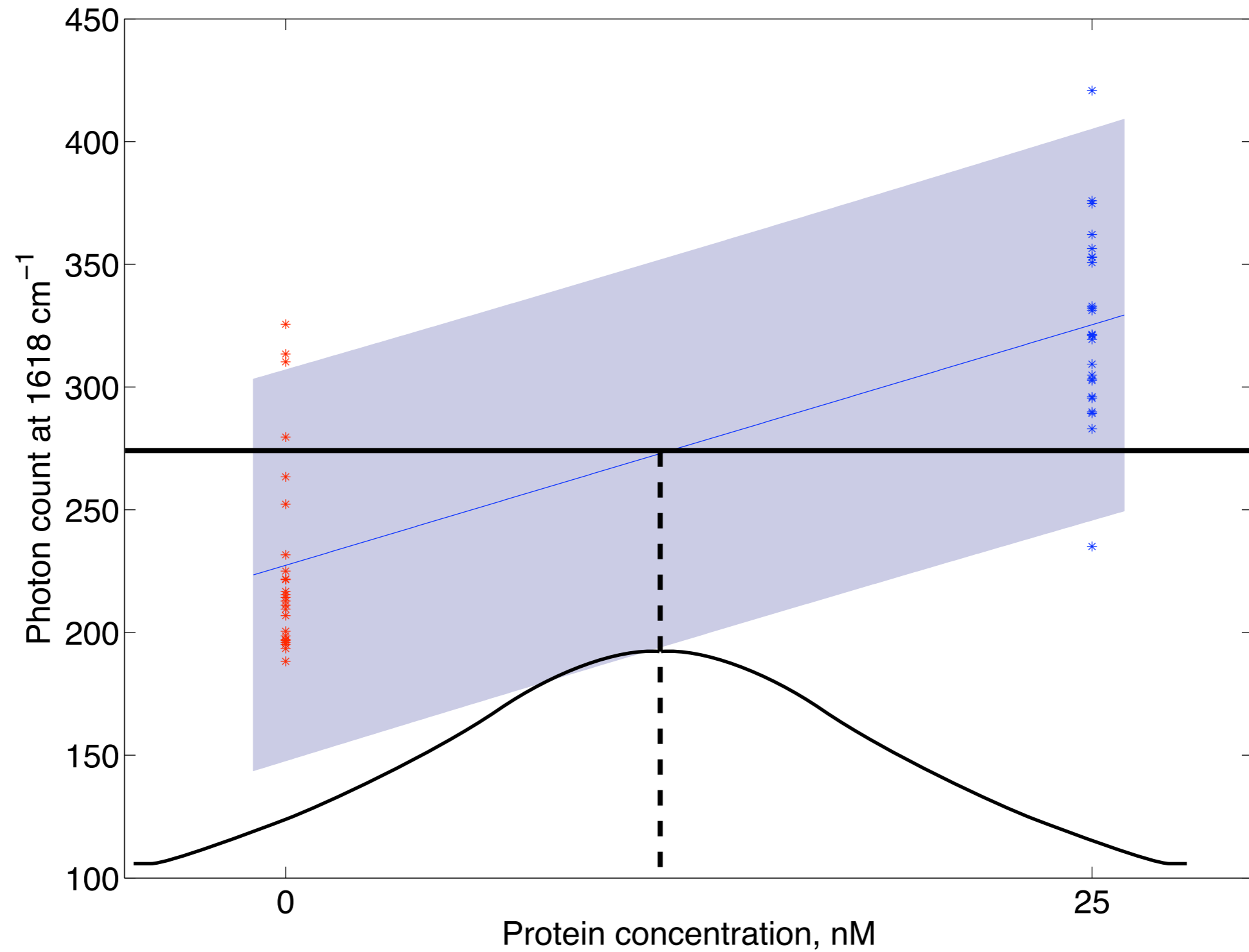
# Can we perform regression?



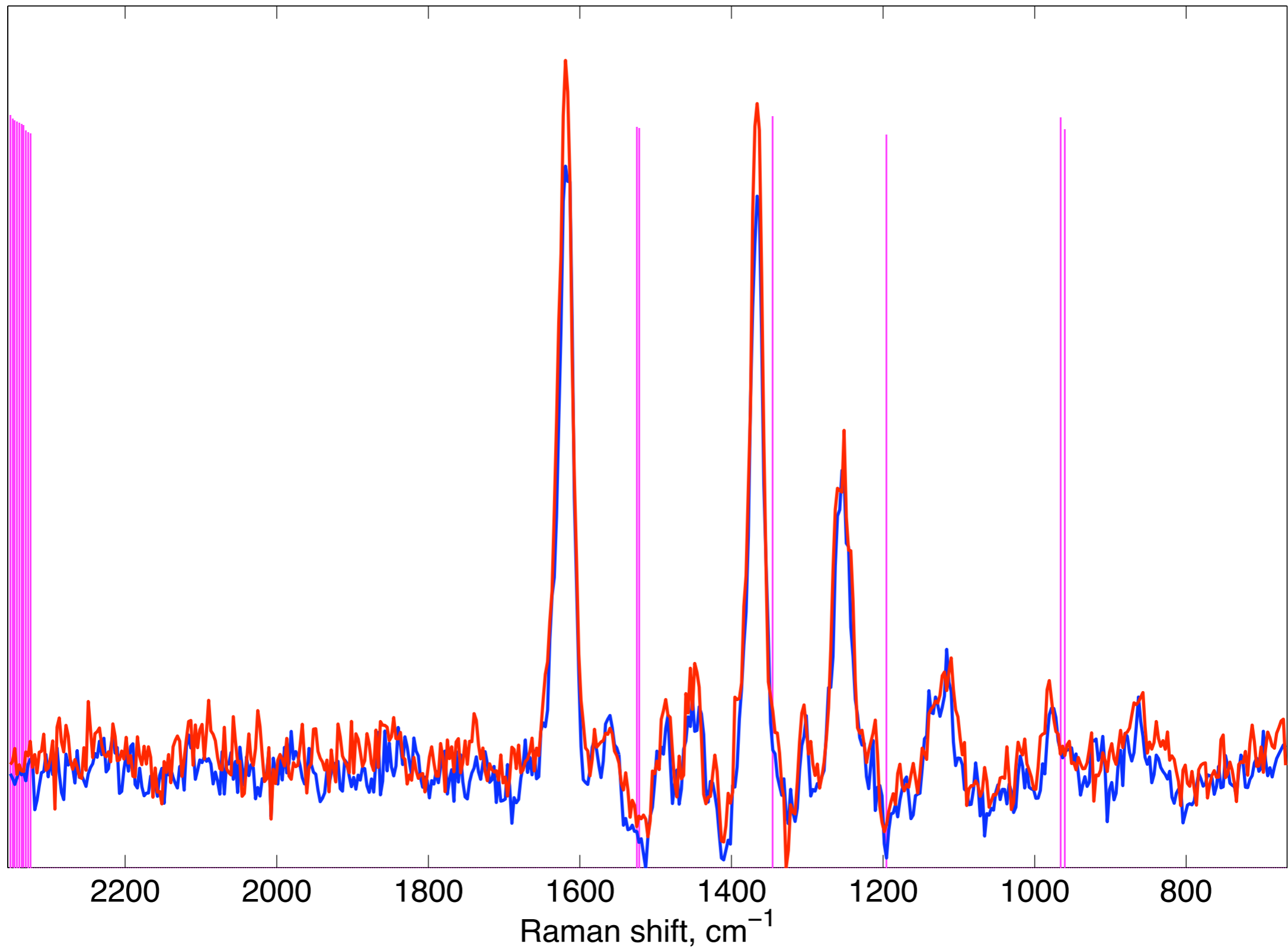
# Can we perform regression?



# Can we perform regression?



# Regularised regression



# Further Work

- The results demonstrate that particle aggregation is happening. No microscopy is required. Publish.
- Finish regularised regression over all of the features, to see if it improves the precision of calibration